

=> fil hcaplus
 FILE 'HCAPLUS' ENTERED AT 16:20:04 ON 06 DEC 2004
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

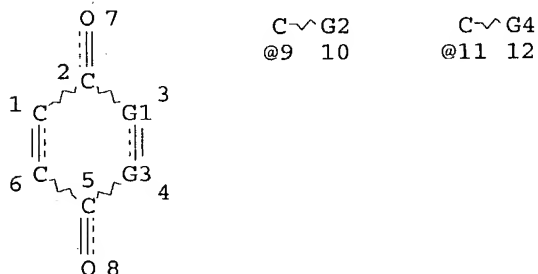
Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 6 Dec 2004 VOL 141 ISS 24
 FILE LAST UPDATED: 5 Dec 2004 (20041205/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
 =>

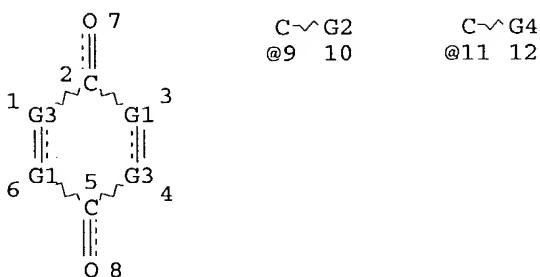
=> d stat que l20
 L7 STR



VAR G1=CH/9
 VAR G2=ME/OH/MEO
 VAR G3=CH/11
 VAR G4=OH/ME/MEO/NO2
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
 L9 SCR 1839
 L11 4180 SEA FILE=REGISTRY SSS FUL L7 NOT L9
 L14 STR



VAR G1=CH/9
 VAR G2=ME/OH/MEO
 VAR G3=CH/11
 VAR G4=OH/ME/MEO/NO2
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L15 901 SEA FILE=REGISTRY SUB=L11 SSS FUL L14
 L16 16802 SEA FILE=HCAPLUS ABB=ON PLU=ON L15
 L18 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L) (?PORIFER? OR ?HELMINTH?
 OR ?COELOMA? OR ?ANNELID? OR ?WORM? OR ?MOLLUSK? OR ?BIVAL?
 OR ?LARV? OR ?COPEPOD? OR ?OSTRACOD? OR ?MYSID? OR ?GAMMARID?
 OR ?DECAPOD? OR ?TELEOS? OR ?STARFISH?)
 L19 361 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L) (PEST? OR AQUACID? OR
 ?VIRUS? OR ?PROTI? OR ?FUNGI? OR MOLD OR MOLDS OR ANTIMOLD OR
 ?PLANKTON? OR ?DEMERS? OR ?BENTHI? OR ?BIOTA? OR ?BACTER? OR
 ?PROTOZO? OR ?ALGAE? OR ?PYRROP? OR ?CRYPTOP? OR ?CHRYSOPH?)
 L20 44 SEA FILE=HCAPLUS ABB=ON PLU=ON (L18 OR L19) AND (WATER OR
 AQUA?)

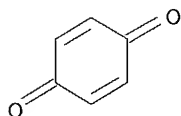
=>
 =>

=> d ibib abs hitstr l20 1-44

L20 ANSWER 1 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2004:69248 HCAPLUS
 DOCUMENT NUMBER: 141:20201
 TITLE: Microbial anaerobic demethylation and dechlorination
 of chlorinated hydroquinone metabolites synthesized by
 basidiomycete fungi
 AUTHOR(S): Milliken, C. E.; Meier, G. P.; Watts, J. E. M.;
 Sowers, K. R.; May, H. D.
 CORPORATE SOURCE: Department of Microbiology and Immunology, Medical
 University of South Carolina, Charleston, SC, USA
 SOURCE: Applied and Environmental Microbiology (2004), 70(1),
 385-392
 CODEN: AEMIDF; ISSN: 0099-2240
 PUBLISHER: American Society for Microbiology
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The synthesis and degradation of anthropogenic and natural organohalides are

the basis of a global halogen cycle. Chlorinated hydroquinone metabolites (CHMs) synthesized by basidiomycete fungi and present in wetland and forest soil are constituents of that cycle. Anaerobic dehalogenating bacteria coexist with basidiomycete fungi in soils and sediments, but little is known about the fate of these halogenated fungal compds. In sediment microcosms, the CHMs 2,3,5,6-tetrachloro-1,4-dimethoxybenzene and 2,3,5,6-tetrachloro-4-methoxyphenol (TCMP) were anaerobically demethylated to tetrachlorohydroquinone (TCHQ). Subsequently, TCHQ was converted to trichlorohydroquinone and 2,5-dichlorohydroquinone (2,5-DCHQ) in freshwater and estuarine enrichment cultures. Screening of several dehalogenating bacteria revealed that Desulfitobacterium hafniense strains DCB2 and PCP1, Desulfitobacterium chlororespirans strain Co23, and Desulfitobacterium dehalogenans JW/DU1 sequentially dechlorinate TCMP to 2,3,5-trichloro-4-methoxyphenol and 3,5-dichloro-4-methoxyphenol (3,5-DCMP). After a lag, these strains demethylate 3,5-DCMP to 2,6-DCHQ, which is then completely dechlorinated to 1,4-dihydroquinone (HQ). 2,5-DCHQ accumulated as an intermediate during the dechlorination of TCHQ to HQ by the TCMP-degrading desulfitobacteria. HQ accumulation following TCMP or TCHQ dechlorination was transient and became undetectable after 14 days, which suggests mineralization of the fungal compds. This is the first report on the anaerobic degradation of fungal CHMs, and it establishes a fundamental role for microbial reductive degradation of natural organochlorides in the global halogen cycle.

IT 106-51-4, Quinone, biological studies
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (microbial anaerobic demethylation and dechlorination of chlorinated
 hydroquinone metabolites synthesized by basidiomycete fungi)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2003:617123 HCAPLUS
 DOCUMENT NUMBER: 139:165586
 TITLE: Porous (meth)acrylic resin material with open cells
 and manufacture of the material
 INVENTOR(S): Misumi, Yoshifumi; Kasahara, Shingo
 PATENT ASSIGNEE(S): Toto Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003226709	A2	20030812	JP 2002-30869	20020207
PRIORITY APPLN. INFO.:			JP 2002-30869	20020207

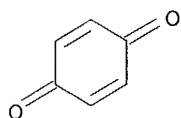
AB The material is that obtained by curing of a composition containing water
 , a surfactant, a polymerization initiator, a crosslinking accelerator, an
 acrylic monomer, and an organic filler mixture of ≥ 1 selected from a
 (meth)acrylic monomer homopolymer, copolymers, and their crosslinked

products. The material is manufactured by the process involving (a) mixing of the components for providing of an emulsion slurry, (b) applying of the slurry into a **water**-nonpermeable mold, (c) demolding of the cured slurry, and (d) removing of residual aqueous solution from the cured product by pressurized air and **water**. Thus, an emulsion containing 520 parts poly(Me methacrylate) (Hipearl D 100M), 156 parts Me methacrylate, polyoxyethylene nonylphenyl ether (Emulgen 930), EtOH, Bz2O2, and N,N-dimethylaniline was molded to give a test piece, in which a slurry corresponding to a ceramic sanitary wear could be cast under only suction without pressure.

IT 106-51-4, p-Benzoquinone, uses
 RL: CAT (Catalyst use); USES (Uses)
 (polymerization inhibitor; for preparation of porous (meth)acrylic resin material with open cells containing organic fillers for ceramic casting mold)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 3 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:108822 HCAPLUS

DOCUMENT NUMBER: 139:311796

TITLE: Bioluminescent bioassays based on luminous bacteria marker system

AUTHOR(S): Kuznetsov, A. M.; Rodicheva, E. K.; Medvedeva, S. E.; Gitelson, J. I.

CORPORATE SOURCE: Institute of Biophysics, Russian Academy of Sciences, Siberian Branch, Krasnoyarsk, 660036, Russia

SOURCE: Bioluminescence & Chemiluminescence: Progress & Current Applications, [Proceedings of the Symposium on Bioluminescence and Chemiluminescence], 12th, Cambridge, United Kingdom, Apr. 5-9, 2002 (2002), 323-326. Editor(s): Stanley, Philip E.; Kricka, Larry J. World Scientific Publishing Co. Pte. Ltd.: Singapore, Singapore.
 CODEN: 69DPGZ; ISBN: 981-238-156-2

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Two bioluminescent bioassays based on lyophilized marine luminous bacteria, Microbiosensor B17-677F, and genetically modified luminous strain of Escherichia coli, Microbiosensor-ECK, were employed to detect zone of impaired **water** quality in the river and sewage **water** of different regions of Siberia. Effect of model substances on Microbiosensor B17-677F compared to its effect on Microbiosensor-ECK showed that in the concentration range evaluated, dependence on the concentration of

the substance was the same. The sensitivity of phenol compds. of the newly developed Microbiosensor-ECK was higher compared to that of Microbiosensor B17-677F. The toxicity of series of phenol compds. produced by Microbiosensor-ECK was in agreement with the toxicity series of phenol compds. determined on intact cells of Photobacterium phosphoreum luminous bacteria and various hydrobionts.

IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, analysis

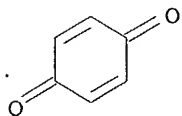
RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)

(bioluminescent bioassays based on luminous **bacteria** marker

system for anal. of river and sewage water)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:42826 HCAPLUS

DOCUMENT NUMBER: 138:68343

TITLE: Biocidal compositions for controlling populations of aquatic pest organisms containing quinones, anthraquinones, and naphthalenediones

INVENTOR(S): Cutler, Stephen J.; Cutler, Horace G.; Wright, David; Dawson, Rodger

PATENT ASSIGNEE(S): Aquacide and Use, USA

SOURCE: U.S. Pat. Appl. Publ., 9 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003012804	A1	20030116	US 2001-886621	20010622
PRIORITY APPLN. INFO.:			US 2001-886621	20010622

OTHER SOURCE(S): MARPAT 138:68343

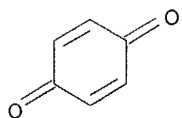
AB Target **aquatic** pest organism populations are controlled by exposing the target population to an effective amount of (a) a biocidal compds. selected from the group consisting of quinones, anthraquinones, naphthalenediones, quinine, warfarin, coumarins, amphotolide, cyclohexadiene-1,4-dione, phenindione, pyridone, sodium rhodizonate, spirulosin and thymoquinone, and (b) a peroxy compound The method is particularly effective for treating ballast **water** of ships or other enclosed vols. of **water** subject to transport between or among geog. areas to control the relocation of plants, toxic bacteria, and animals contained in the **water**.

IT 106-51-4D, Cyclohexadiene-1,4-dione, mixts. with peroxy compds.
 319-89-1D, Tetrahydroxy-p-benzoquinone, mixts. with peroxy compds.
 479-22-1D, mixts. with peroxy compds. 484-89-9D,
 3-Hydroxy-2-methoxy-5-methyl-p-benzoquinone, mixts. with peroxy compds.
 530-55-2D, mixts. with peroxy compds. 553-97-9D, mixts.
 with peroxy compds. 605-94-7D, mixts. with peroxy compds.

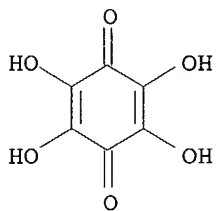
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
 (biocidal compds. for controlling populations of **aquatic pest** organisms containing)

RN 106-51-4 HCAPLUS

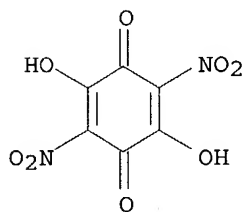
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



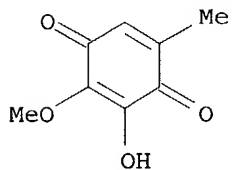
RN 319-89-1 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy- (9CI) (CA INDEX NAME)



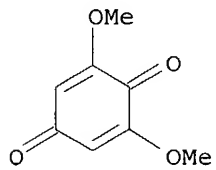
RN 479-22-1 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3,6-dinitro- (9CI) (CA INDEX NAME)



RN 484-89-9 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)

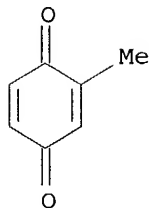


RN 530-55-2 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)



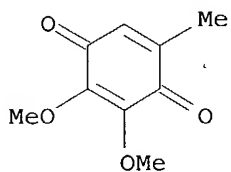
RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



L20 ANSWER 5 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:42257 HCAPLUS

DOCUMENT NUMBER: 138:106698

TITLE: Preparation of 4-arylquinols and analogs thereof as antiproliferative agents, anticancer agents, antimycobacterial agents, antituberculosis agents, and/or thioredoxin/thioredoxin reductase inhibitors

INVENTOR(S): Stevens, Malcolm Francis Graham; Wells, Geoffrey; Westwell, Andrew David; Poole, Tracey Dawn

PATENT ASSIGNEE(S): Cancer Research Technology Limited, UK

SOURCE: PCT Int. Appl., 180 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003004479	A1	20030116	WO 2002-GB3097	20020705
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1404659	A1	20040407	EP 2002-745585	20020705
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
JP 2004533486	T2	20041104	JP 2003-510646	20020705

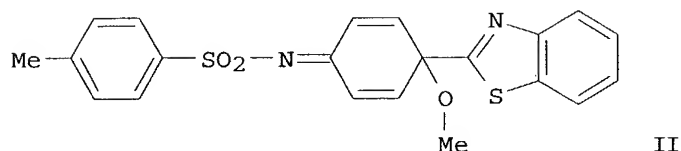
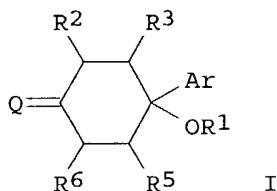
US 2004220236
PRIORITY APPLN. INFO.:

A1 20041104
MARPAT 138:106698

US 2004-482912
GB 2001-16594
WO 2002-GB3097

20040427
A 20010706
W 20020705

OTHER SOURCE(S):
GI



AB The present invention pertains to compds. of the formula (I) (wherein: Q is O or :NSO₂R; R is H or optionally substituted C1-7 alkyl, C3-20 heterocyclyl, or C5-20 aryl; Ar is optionally substituted C5-20 aryl; R1 is H or an oxy substituent such as optionally substituted C1-7 alkyl, C3-20 heterocyclyl, C5-20 heterocyclyl, C5-20 aryl, C1-7 alkylacyl, C3-20 heterocyclyl-acyl, or C5-20 aryl-acyl; the bond marked α is a single bond or a double bond; the bond marked β is a single bond or a double bond; R3 and R5 are each independently ring substituents; R2 and R6 are each independently ring substituents) and pharmaceutically acceptable salts, esters, amides, solvates, hydrates, and protected forms thereof. The present invention also pertains to pharmaceutical compns. comprising the compds. I, and the use of the compds. I and compns., both in vitro and in vivo, for example, in the treatment of proliferative conditions, (e.g., cancer), mycobacterial infections (e.g., tuberculosis), and/or conditions mediated by thioredoxin/thioredoxin reductase. These compds. I are useful as antiproliferative agents, anticancer agents, antimycobacterial agents, antituberculosis agents, and/or thioredoxin/thioredoxin reductase inhibitors (no data). Thus, to 0.5 g 2-(4-aminophenyl)benzothiazole in 6 mL pyridine was added 0.506 g p-toluenesulfonyl chloride in 4 mL pyridine, heated at reflux for 10 min, cooled, and treated with 10 mL water to 96% N-[(4-benzothiazol-2-yl)phenyl]-4-methylbenzenesulfonamide which (0.1 g) was dissolved in 2 mL MeOH and stirred with BTIB (1.1 15 equivalent) at room temperature for 5 h to give 73% N-[4-methoxy-4-(benzothiazol-2-yl)cyclohexa-2,5-dienylidene]-4-methylbenzenesulfonamide (II). 4-(Benzothiazol-2-yl)-4-hydroxy-2,5-cyclohexadien-1-one in vitro showed IC₅₀ of 0.04, 0.38, 0.35, 0.79, and 2.35 μM for inhibiting the proliferation of HCT and HT29 human colon carcinoma, human MCF-7 and MDA, 468 breast carcinoma, and A549 human lung adenocarcinoma, resp.

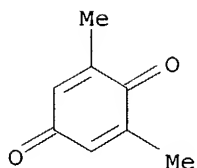
IT 527-61-7, 2,6-Dimethyl-1,4-benzoquinone

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; preparation of 4-arylquinols and analogs thereof as antiproliferative agents, anticancer agents, **antimycobacterial** agents, antituberculosis agents, and/or thioredoxin/thioredoxin reductase inhibitors)

RN 527-61-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 6 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:556093 HCAPLUS

DOCUMENT NUMBER: 137:105181

TITLE: Pesticide for control of aquatic pests in ballast water of ships

INVENTOR(S): Cutler, Stephen J.; Cutler, Horace G.; Wright, David; Dawson, Rodger

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 11 pp., Cont.-in-part of U.S. Ser. No. 506,017.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002098979	A1	20020725	US 2001-3465	20011206
<u>US 6340468</u>	B1	20020122	US 2000-506017	20000217
US 2002098978	A1	20020725	US 2001-3464	20011206
US 6576674	B2	20030610		

PRIORITY-APPLN. INFO.: US 2000-506017 A2 20000217
US 2000-237401P P 20001004

OTHER SOURCE(S): MARPAT 137:105181

AB The title pesticides are quinones, anthraquinones, naphthalenediones, quinine, warfarin, coumarins, amphotolide, cyclohexadiene-1,4-dione, phenindione, sodium rhodizionate, apirulosin and thymoquinone. The method is particularly effective for treating ballast water of ships or other enclosed vols. of water subject to transport between or among geog. areas to control the relocation of plants, toxic bacteria, and animals contained in the water. The method is especially useful to control zebra mussels in the ballast waters.

IT 106-51-4, 1,4-Benzoquinone, biological studies 319-89-1,

Tetrahydroxy-p-benzoquinone 479-22-1, p-Benzoquinone-,

2,5-Dihydroxy-3,6-dinitro 484-89-9, p-Benzoquinone-,

3-hydroxy-2-methoxy-5-methyl 530-55-2 553-97-9

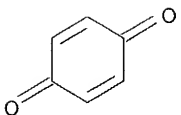
605-94-7, 2,3-Dimethoxy-5-methyl-1,4-Benzoquinone

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

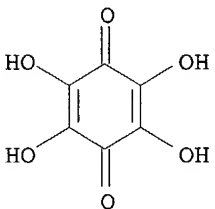
(pesticide for control of aquatic pests in ballast water of ships)

RN 106-51-4 HCAPLUS

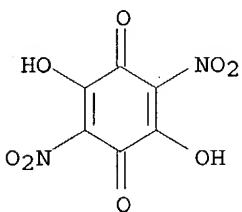
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



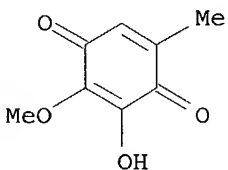
RN 319-89-1 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy- (9CI) (CA INDEX NAME)



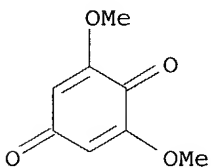
RN 479-22-1 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3,6-dinitro- (9CI) (CA INDEX NAME)



RN 484-89-9 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)

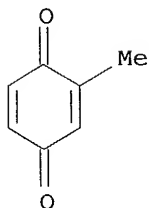


RN 530-55-2 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)



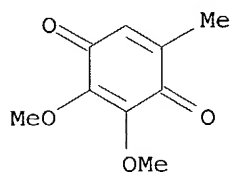
RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



L20 ANSWER 7 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:859502 HCAPLUS

DOCUMENT NUMBER: 136:270312

TITLE: Photochemical behavior of 4-chloro-2-methylphenoxyacetic acid Influence of pH and irradiation wavelength

AUTHOR(S): Zertal, Abdenmour; Sehili, Tahar; Boule, Pierre

CORPORATE SOURCE: Departement de Chimie, Laboratoire des Sciences et Technologie de l'Environnement, Faculte des Sciences, Universite de Constantine, Constantine, 25000, Algeria

SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (2001), 146(1-2), 37-48
CODEN: JPPCEJ; ISSN: 1010-6030

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The kinetics of phototransformation of 4-chloro-2-methylphenoxyacetic acid (MCPA) is studied under various irradiation conditions. The photocatalytic transformation on TiO₂ in aqueous suspension is almost specific and leads to 4-chloro-2-methylphenol (P7) as the main photoproduct. The same product is obtained when MCPA is irradiated on silica in the absence of **water**. The direct phototransformation is more complex: the reaction is not influenced by oxygen but it depends on the pH of the solution and on the irradiation wavelength. With the anionic form irradiated between 254 and 350 nm, photohydrolysis of C-Cl bond is almost quant. (yield >86%). It leads to the hydroxylated photoproduct P2. With the mol. form the main product P5 results from a photochem. rearrangement of the mol. With both forms, some other photoproducts are also identified and quantified, particularly methylhydroquinone (P1) and P7, 2-methylphenol (P6) is only obtained with the anionic form as a minor product. However, irradiation of solns. in sunlight or with lamps emitting mainly at 365 nm (about 2 and 6% of the light is emitted at 334 and 313 nm, resp.) yields P7 as the main photoproduct. Its formation is self-accelerated. This wavelength effect is attributed to reactions induced by quinonic compds. formed as intermediates since the disappearance of MCPA is more efficient

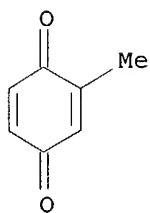
in presence of quinonic products. P7 is also the major photoproduct when phototransformation is induced by nitrite ions or Fe(III) perchlorate. Besides, it appears from Microtox test that photoproducts formed at wavelength shorter than 350 nm are more toxic to the marine bacterium *Vibrio fischeri* than the initial compound

IT 553-97-9P

RL: ADV (Adverse effect, including toxicity); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(photoproduct; photochem. of chloromethylphenoxyacetic acid as function of pH and irradiation wavelength and evaluation of photoproducts toxicity to marine bacterium *Vibrio fischeri*)

RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 8 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:626671 HCAPLUS

DOCUMENT NUMBER: 136:8952

TITLE: Photosynthetic bioelectrochemical cell utilizing

cyanobacteria and water-generating oxidase

AUTHOR(S): Tsujimura, S.; Wadano, A.; Kano, K.; Ikeda, T.

CORPORATE SOURCE: Graduate School of Agriculture, Division of Applied Life Sciences, Kyoto University, Sakyo, Kyoto, 606-8502, Japan

SOURCE: Enzyme and Microbial Technology (2001), 29(4-5), 225-231

CODEN: EMTED2; ISSN: 0141-0229

PUBLISHER: Elsevier Science Ireland Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

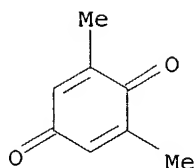
AB A novel photosynthetic bioelectrochem. cell that utilizes biocatalysts in both anode and cathode compartments was constructed for the first time. in the anodic half-cell, some parts of the electrons produced by the oxidation of water in the photosystem of cyanobacteria are transferred to the carbon felt anode through quinonoid electron transfer mediators. The electron is passed to dioxygen to regenerate water in the cathodic half-cell reaction with an aid of bilirubin oxidase reaction via a mediator. The maximum elec. power was about 0.3-0.4 W m⁻² for the projective electrode surface area at an apparent efficiency of the light energy conversion of 2-2.5%. The factors governing the cell output are discussed on the basis of the potential-current curves of each half-cell.

IT 527-61-7, 2,6-Dimethyl-1,4-benzoquinone

RL: DEV (Device component use); USES (Uses)
(photosynthetic bioelectrochem. cell utilizing cyanobacteria and water-generating oxidase)

RN 527-61-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 9 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:618136 HCAPLUS

DOCUMENT NUMBER: 135:191666

TITLE: Biocidal compds. for controlling populations of aquatic pest organisms containing quinones, anthraquinones, and naphthalenediones

INVENTOR(S): Cutler, Horace; Cutler, Stephen; Wright, David; Dawson, Rodger

PATENT ASSIGNEE(S): Garnett, Inc., USA

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

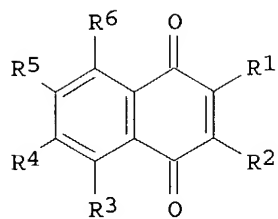
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

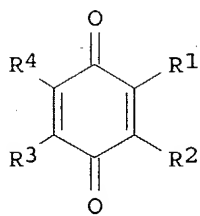
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001060971	A2	20010823	WO 2001-US5117	20010216
WO 2001060971	A3	20011213		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, FR, GB, GD, GE, GH, GM, GR, GU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OL, OM, OS, PA, PE, PG, PH, PI, PL, PT, PU, PZ, RE, RO, RU, SD, SE, SG, SI, SK, SL, SM, SN, SR, ST, SV, SW, SY, SZ, TC, TD, TF, TG, TH, TJ, TM, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6340468	B1	20020122	US 2000-506017	20000217
CA 2406968	AA	20010823	CA 2001-2406968	20010216
AU 2001041530	A5	20010827	AU 2001-41530	20010216
EP 1261254	A2	20021204	EP 2001-912784	20010216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003523821	T2	20030812	JP 2001-560343	20010216
EE 200200455	A	20031215	EE 2002-455	20010216
US 2002098978	A1	20020725	US 2001-3464	20011206
US 6576674	B2	20030610		
NO 2002003912	A	20021007	NO 2002-3912	20020816
BG 107108	A	20030430	BG 2002-107108	20020916
PRIORITY APPLN. INFO.:				
			US 2000-506017	A 20000217
			US 2000-237401P	P 20001004
			WO 2001-US5117	W 20010216

OTHER SOURCE(S): MARPAT 135:191666

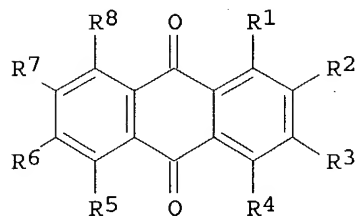
GI



I



II



III

AB Biocidal compds. for controlling populations of **aquatic** pest microorganisms, plants or animals are selected from the group consisting of naphthalenediones I (R1 = H, OH, Me; R2 = H, Me, sodium bisulfate, Cl, acetonyl, 3-methyl-2-butenyl, 2-oxypropyl; R3 = H, Me, Cl, methoxy, or 3-methyl-2-butenyl; R4 = H, methoxy; R5 = H, OH, Me; R6 = H, OH), quinones II (R1 = H, Me, OH, methoxy; R2 = H, OH, Me, methoxy, NO2; R3 = H, OH, Me, methoxy; R4 = H, Me, methoxy, OH, NO2), anthraquinones III (R1 = H, OH, Cl; R2 = H, Me, Cl, OH, carbonyl, carboxyl; R3 = H, Me; R4 = H; R5 = H, OH; R6, R7 = H; R8 = H, OH), quinine, warfarin, coumarins, amphotalide, cyclohexadiene-1,4-dione, phenidione, pirdone, sodium rhodizonate, apirulosin, thymoquinone, . The compds. are used to control population of target pest microorganisms is selected from the group consisting of viruses, protists, holoplanktonic organisms, and meroplanktonic organisms, demersal organisms, benthic organisms, detached or floating biota, bacteria, encysted bacteria, protozoans, algae, pyrrophyta, cryptophyta, chrysophyta, porifera, platyhelminthes, pseudocoelomates, annelid worms, zebra mussels, bivalves, larval forms of copepods, ostracods, mysids, gammarids, larval forms of decapods, and larval teleost fish. The method is particularly effective for treating ballast **water** of ships or other enclosed vols. of **water** subject to transport between or among geog. areas to control the relocation of plants, bacteria, and animals contained in the **water**.

IT 106-51-4, Cyclohexadiene-1,4-dione, biological studies

319-89-1, Tetrahydroxy-p-benzoquinone 479-22-1

484-89-9, 3-Hydroxy-2-methoxy-5-methyl-p-benzoquinone

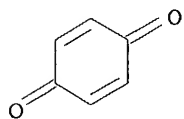
530-55-2 553-97-9 605-94-7

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(biocidal compds. for controlling populations of **aquatic** pest organisms containing)

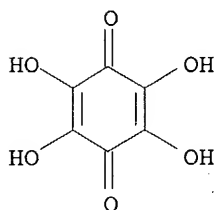
RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



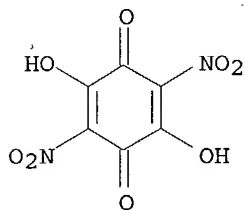
RN 319-89-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy- (9CI) (CA INDEX NAME)



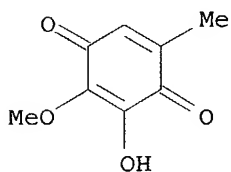
RN 479-22-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3,6-dinitro- (9CI) (CA INDEX NAME)



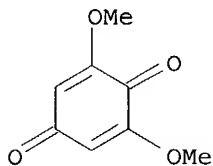
RN 484-89-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)



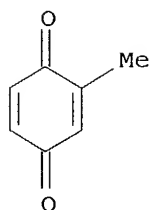
RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)

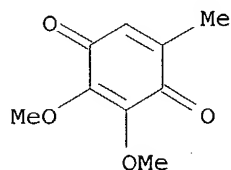


RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



RN 605-94-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



L20 ANSWER 10 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:109589 HCAPLUS

DOCUMENT NUMBER: 134:359368

TITLE: Electrochemical investigation of cyanobacteria
 Synechococcus sp. PCC7942-catalyzed photoreduction of
 exogenous quinones and photoelectrochemical oxidation
 of **water**

AUTHOR(S): Torimura, M.; Miki, A.; Wadano, A.; Kano, K.; Ikeda,
 T.

CORPORATE SOURCE: Division of Applied Life Sciences, Graduate School of
 Agriculture, Kyoto University, Kyoto, Sakyo, 606-8502,
 Japan

SOURCE: Journal of Electroanalytical Chemistry (2001),
 496(1-2), 21-28

CODEN: JECHES; ISSN: 0368-1874

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electron transfer from the photosynthetic system in cyanobacteria,
 Synechococcus sp. PPC7942 to exogenous electron acceptors was examined using
 several electrochem. techniques. 1,4-Benzoquinone (BQ) and
 2,6-dimethyl-1,4-benzoquinone (DMBQ) were found to function as good
 exogenous electron acceptors for the photosystem. Kinetic anal. with
 rotating disk amperometry revealed that the photoredn. of these quinones
 proceeds in Michaelis-Menten type kinetics for the concentration of the quinones
 and the light intensity. The electron transfer rate of the BQ reduction was
 as high as 68% compared with that of the photosynthetic oxygen evolution.
 Synechococcus sp. cell-entrapped and DMBQ-embedded carbon paste electrodes
 provided steady-state current ascribed to the photoelectrochem. oxidation of
water. Although several inhibitors against the photosynthetic
 system suppressed the photoelectrochem. response, phenylmercury acetate,
 which inhibits ferredoxin and ferredoxin-NADP oxidoreductase, was found to
 enhance the photocurrent. Some electrochem. aspects of this system are
 discussed.

IT 106-51-4, 1,4-Benzoquinone, reactions 527-61-7,
 2,6-Dimethyl-1,4-benzoquinone

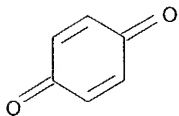
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC

(Process); RACT (Reactant or reagent)

(electrochem. investigation of **cyanobacteria** *Synechococcus* sp. PCC7942 catalyzed photoredn. of exogenous quinones and photoelectrochem. oxidation of **water**)

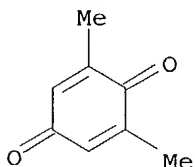
RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 527-61-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 11 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:773826 HCAPLUS

DOCUMENT NUMBER: 134:96495

TITLE: Sediment mutagenicity testing: Development of substance specific bacterial strains for the detection of mutagenic aromatic nitrogen compounds and oxidative mutagens

AUTHOR(S): Vahl, H. H.; Karbe, L.; Prieto-Alamo, M. J.; Pueyo, C.; Westendorf, J.

CORPORATE SOURCE: Department of Toxicology, Medical School, University of Hamburg, Hamburg, D-22527, Germany

SOURCE: Aquatic Ecosystem Health & Management (2000), 3(3), 360-378

CODEN: AEHMF4; ISSN: 1463-4988

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The arabinose resistance forward mutation assay was chosen for the development of bacterial strains in order to get specific mutagenic responses. Special strains of *Salmonella typhimurium* were constructed which show an elevated expression of nitroreductase and O-acetyltransferase. They were shown to be highly sensitive to mutagenic nitro-compds. (e.g. 1-nitropyrene and 1,8-dinitropyrene) and, after metabolic activation by rat liver S9-mix, also to mutagenic amino-compds. (2-aminoanthracene). Furthermore, strains of *Escherichia coli* with reduced expression of antioxidative enzymes (catalase and superoxide dismutase) were constructed. However, they were only moderately sensitive to oxidative mutagens such as quinones, nitrogen compds., and the herbicide paraquat, because, in contrast to the *Salmonella* strains used, they build up a complete gram-neg. cell wall. For this reason, the *Escherichia* strains were further genetically altered in order to make their cell wall penetrable to lipophilic compds. This alteration increased the sensitivity to more lipophilic compds. The strains were

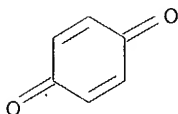
more sensitive to 1-nitropyrene by a factor of more than 10 and to 1,8-dinitropyrene by a factor of more than 100. In order to validate the arabinose resistance test with the newly constructed strains, sediments of the whole German part of the Elbe River were examined. Overall mutagenicity (standard strains) as well as enhanced effects with the special strains were observed in sediment samples of the river. Mutagenic hot spots reflect direct industrial influences as well as hydrol. situations, which has led to concentration of the organic content of suspended matter, loaded with industrial or rural contamination. Generally, high mutagenic effects were observed where chemical analyses showed a high degree of contamination.

IT 106-51-4, Quinone, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(sediment mutagenicity testing and development of substance specific
bacterial strains for the detection of mutagenic aromatic nitrogen
comps. and oxidative mutagens).

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 12 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:213642 HCAPLUS

DOCUMENT NUMBER: 132:212299

TITLE: Quinone profiles in lake sediments: implications for
microbial diversity and community structures

AUTHOR(S): Hiraishi, Akira; Kato, Kenji

CORPORATE SOURCE: Department of Ecological Engineering, Toyohashi
University of Technology, Toyohashi, 441-8580, Japan

SOURCE: Journal of General and Applied Microbiology (1999),
45(5), 221-227

CODEN: JGAMA9; ISSN: 0022-1260

PUBLISHER: Microbiology Research Foundation

DOCUMENT TYPE: Journal

LANGUAGE: English

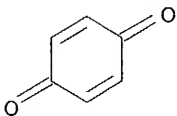
AB Microbial quinone comps. of sediment mud samples from 5 lakes in Japan were studied by spectro-chromatog. and mass spectrometry. Total quinone content of these samples was 1.97-18.0 nmol/g dry weight sediment, of which a combined fraction of ubiquinones and menaquinones accounted for 42-74%. The remaining fraction (26-58%) consisted of the photosynthetic quinones, plastoquinones and phylloquinone. Sediment samples produced PQ-9 or Q-8 as the most abundant quinone type regardless of their geog. location and depth. Results indicated that oxygenic phototrophic microorganisms and Q-8-containing proteobacteria constituted major parts of microbial populations in lake sediment. In surface **water** of the same sampling sites, plastoquinones and phylloquinone occurred in much higher proportions. These findings suggested the abundance of oxygenic phototrophs in sediment muds resulted from their constant movement or sedimentation from the surface **water**. Numerical analyses of quinone profiles showed that sediment microbial communities were diverse and different in different lakes, but similar to each other in the diversity of bio-energetic modes. Three physiol. groups of microbes exhibiting ubiquinone-mediated aerobic respiration, oxygenic photosynthesis, and menaquinone-associated respiration, were suggested to inhabit the lake sediment in balance.

IT 106-51-4, Quinone, biological studies

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); OCU (Occurrence, unclassified); BIOL (Biological study); OCCU (Occurrence) (bacterial; lake sediment quinone profiles and their implication for microbial diversity and community structures)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 13 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:385535 HCAPLUS

DOCUMENT NUMBER: 131:155862

TITLE: Investigation on the detergent role in the function of secondary quinone in bacterial reaction centers

AUTHOR(S): Agostiano, Angela; Milano, Francesco; Trotta, Massimo

CORPORATE SOURCE: Dipartimento di Chimica, Universita di Bari, Bari, I-70126, Italy

SOURCE: European Journal of Biochemistry (1999), 262(2), 358-364

CODEN: EJBCAI; ISSN: 0014-2956

PUBLISHER: Blackwell Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In this paper are reported studies on the detergent role in isolated reaction centers (RC) from Rhodobacter sphaeroides, over a large range of lauryldimethylamino-N-oxide (LDAO) concns., in influencing the thermodyn. of the quinone exchange reaction as well as the protein aggregation. The occurrence of the quinone exchange reaction between the QB-binding site (where QB is the second quinone mol. of two in the RC) and the ubiquinone 0 dissolved in the different environments (water, LDAO micelles and detergent phase of the protein-detergent complex) has also been analyzed. Measurements carried out in QB-depleted RC to which exogenous quinone has been added show that the relative amplitudes of the slow and fast phase of the recombination reaction depend on this parameter. The overall amount of the restored QB-functionality is affected by the concentration of the LDAO in solution. Interpolation of the titration curves with a quadratic function obtained by simple considerations allowed the binding constant of UQ0 to the QB-binding site to be calculated. From the fitting procedure, the distribution of the quinone in the different environments present in solution was evaluated, indicating that the exchange reaction can take place only between the QB-site and the detergent phase. The dependence of the quinone pool size upon the volume of the phase in which the interacting quinone is solubilized is also discussed. The increasing difficulty in saturating the QB-pocket above the LDAO critical micellar concentration is finally related to the association of protein-detergent complexes to form large protein clusters.

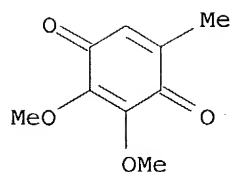
IT 605-94-7, Ubiquinone 0

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(detergent role in the function of secondary quinone in bacterial reaction centers)

RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 14 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:573580 HCAPLUS

DOCUMENT NUMBER: 125:214499

TITLE: Benzo[a]pyrene metabolism and xenobiotic-stimulated reactive oxygen species generation by subcellular fraction of larvae of turbot (*Scophthalmus maximus* L.)

AUTHOR(S): Peters, L. D.; O'Hara, S. C. M.; Livingstone, D. R.

CORPORATE SOURCE: NERC Plymouth Marine Laboratory, Devon, PL1 2PB, UK

SOURCE: Comparative Biochemistry and Physiology, C: Pharmacology, Toxicology and Endocrinology (1996), 114C(3), 221-227

CODEN: CBPCEE; ISSN: 0742-8413

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

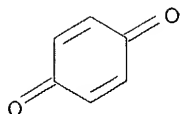
AB NADPH-dependent 3H-benzo[a]pyrene (BaP) metabolism and basal and xenobiotic-stimulated NAD(P)H-dependent reactive oxygen species (ROS) production were investigated in 11,600 g supernatants of 4-day-old (yolk sac) larvae of turbot (*Scophthalmus maximus* L.). BaP metabolites were resolved by HPLC and detected radiometrically. ROS were quantified by the iron-EDTA mediated production of hydroxyl radical ($\cdot\text{OH}$) that was detected by its oxidation of 2-keto-4-methiobutyric acid (KMBA) to yield ethylene. BaP metabolism produced phenols, dihydrodiols and diones (quinones) (resp., 54, 32, and 14% of free metabolites) and putative protein adducts. Metabolites identified by retention time included the 7,8-dihydrodiol, the 1,6-, 3,6- and 6,12-diones and the 3- and 9-phenols. Pre-exposure of turbot larvae to 5 ppb BaP for 24 h caused an approx. 2-fold increase in both BaP metabolism and 7-ethoxyresorufin O-deethylase activity, indicative of the induction of cytochrome P 4501A and its involvement in BaP metabolism. Basal KMBA oxidation rates were similar for NADH and NADPH. Inhibition studies indicate that $\cdot\text{OH}$ was formed via the production of superoxide anion radical and hydrogen peroxide. Basal ROS production was stimulated up to 3-fold by a range of redox cycling aromatic hydrocarbon quinones and indicated to be stimulated by other xenobiotics, including nitroaroms. The results indicate biotransformation and ROS production as potential mechanisms of toxicity in larval fish.

IT 106-51-4, 1,4-Benzquinone, biological studies 527-17-3, Duroquinone

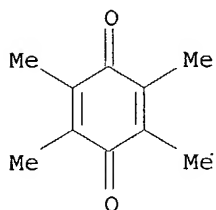
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(benzopyrene metabolism and xenobiotic-stimulated reactive oxygen species generation by subcellular fraction of larvae of turbot)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 527-17-3 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)



L20 ANSWER 15 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:101103 HCAPLUS

DOCUMENT NUMBER: 116:101103

TITLE: Reduction of ethylenethiourea content in
 alkylenebisdithiocarbamate fungicides, using
 hydroxymethane sulfinat

INVENTOR(S): Diepenhorst, Pieter Carel; Kool, Pieter; Nouws,
 Jacobus Adrianus Maria

PATENT ASSIGNEE(S): Atochem Agri S. A., Fr.

SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 460612	A1	19911211	EP 1991-109126	19910604
EP 460612	B1	19950510		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5100915	A	19920331	US 1990-533967	19900606
AU 9178045	A1	19911212	AU 1991-78045	19910530
AU 640233	B2	19930819		
JP 04235957	A2	19920825	JP 1991-159498	19910604
JP 2872448	B2	19990317		
AT 122206	E	19950515	AT 1991-109126	19910604
ES 2071862	T3	19950701	ES 1991-109126	19910604
BR 9102335	A	19920107	BR 1991-2335	19910605
			US 1990-533967	A 19900606

PRIORITY APPLN. INFO.:

AB A method is provided for stabilizing alkylenebisdithiocarbamates, such as 1,2-ethylenebisdithiocarbamates (EBDC), by mixing the EBDC in the presence of **water** with hydroxymethanesulfinat (HMS) which degrades to HCHO to reduce the content of ethylenethiourea (ETU) in the EBDC. The HMS and sulfite byproduct from the HCHO formation also act as reducing agents to inhibit further ETU formation by oxidative decomposition of EBDC. The HMS is preferably added at 0.1-5% by weight, based upon the EBDC, and the aqueous reaction mixture is then preferably dried under vacuum. Copolymn. agents, such as hydroquinone or melamine, may also be added to further reduce and inhibit ETU formation. Mancozeb (4 g) was treated with 50 mg HMS Na salt

and 10 mL water, followed by drying. After 45 days, the ETU content was decreased to 0.01% from the original 0.05%.

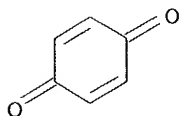
IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies

RL: BIOL (Biological study)

(alkylenebisdithiocarbamate fungicides stabilization by hydroxymethanesulfinate and, decrease in ethylenethiourea content in relation to)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 16 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:625722 HCAPLUS

DOCUMENT NUMBER: 115:225722

TITLE: Quantitative structure-activity relationships for chemical toxicity to environmental bacteria

AUTHOR(S): Blum, Diane J. W.; Speece, R. E.

CORPORATE SOURCE: Bala Cynwyd, PA, 19004, USA

SOURCE: Ecotoxicology and Environmental Safety (1991), 22(2), 198-224

CODEN: EESADV; ISSN: 0147-6513

DOCUMENT TYPE: Journal

LANGUAGE: English

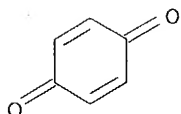
AB QSARs were developed for nonreactive chemical toxicity to each of four groups of bacteria of importance in environmental engineering: aerobic heterotrophs, methanogens, Nitrosomonas, and Microtox. The QSARs were based on chems. covering a range of structures and including important environmental pollutants (i.e., chlorinated and other substituted benzenes, phenols, and aliphatic hydrocarbons). QSARs were developed for each chemical class and for combinations of chemical classes. Three QSAR methods (groups of chemical describing parameters) were evaluated for their accuracy and ease of use: log P, linear solvation energy relationships (LSER), and mol. connectivity. Successful QSARs were found for each group of bacteria and by each method, with correlation coeffs. (adjusted r²) between 0.79 and 0.95. LSER QSARs incorporated the widest range of chems. with the greatest accuracy. Log P and mol. connectivity QSARs are easier to use because their parameters are readily available. Outliers from the QSARs likely due to reactive toxicity included acryls, low pK_a compds., and aldehydes. Nitro compds. and chlorinated aliphatic hydrocarbons and alcs. showed enhanced toxicity to the methanogens only. Chems. with low IC₅₀ concns. (log IC₅₀ μmol/L < 1.5) were often outliers for Nitrosomonas. QSARs were validated statistically and with literature data. A suggested method is provided for use of the QSARs.

IT 106-51-4, 1,4-Benzoquinone, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to environmental bacteria, mol. structure effect on)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 17 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:147323 HCAPLUS

DOCUMENT NUMBER: 108:147323

TITLE: Characterization of protonmotive force generation in liposomes reconstituted from phosphatidylethanolamine, reaction centers with light-harvesting complexes isolated from *Rhodospseudomonas palustris*

AUTHOR(S): Molenaar, Douwe; Crielard, Wim; Hellingwerf, Klaas J.

CORPORATE SOURCE: Dep. Microbiol., Univ. Groningen, Haren, 9751 NN, Neth.

SOURCE: Biochemistry (1988), 27(6), 2014-23

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reaction center complexes were isolated from *R. palustris* with either one or both of the light-harvesting complexes attached. Both complexes were incorporated into liposomes made of phospholipids purified from *Escherichia coli*. Light-driven cyclic electron transport could be restored in these proteoliposomes upon the addition of the redox mediators cytochrome c and a water-soluble ubiquinone. During cyclic electron transport in this artificial system, protons are extruded electrogenically from the liposomes, and this leads to the generation of a protonmotive force (PMF). The optimal conditions for PMF generation were pH 8, a reaction center/lipid ratio of 1.4 nmol/mg, and cytochrome c and ubiquinone 0 concns. of 10 and 400 μ M, resp. The maximum membrane potential generated under these conditions was -180 mV. From titration studies with a protonophore, it was found that the intrinsic maximum capacity of the reaction centers in PMF generation (the electromotive force) equals -210 mV.

No evidence was obtained for a contribution of light-harvesting complex II to PMF generation; i.e., these complexes are functionally uncoupled from the reaction centers. Neither was an electrochromic band shift of the carotenoids, present in these complexes, measurable upon illumination. A kinetic model representing the artificial redox chain cytochrome c/reaction center/ubiquinone 0 is presented. For this model, data have been used from fast kinetic studies on reaction centers from *Rhodobacter sphaeroides*. The model explains the observed discrepancy between the dissociation constant (K_d) of reaction centers for cytochrome c and the Michaelis constant (K_m) for the rate of cytochrome c oxidation. The model also explains the light dependency of this K_m .

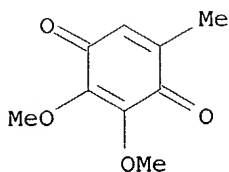
IT 605-94-7, Ubiquinone 0

RL: BIOL (Biological study)

(reconstituted liposomes containing **bacterial** reaction centers and, protonmotive force generation in relation to)

RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



L20 ANSWER 18 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:105130 HCAPLUS
 DOCUMENT NUMBER: 106:105130
 TITLE: Coal extraction by aprotic dipolar solvents
 AUTHOR(S): Sears, J. T.
 CORPORATE SOURCE: Montana State Univ., Bozeman, MT, USA
 SOURCE: Report (1985), DOE/PC/50787-T6; Order No. DE86005354, 175 pp. Avail.: NTIS
 From: Energy Res. Abstr. 1986, 11(8), Abstr. No. 15507
 DOCUMENT TYPE: Report
 LANGUAGE: English

AB The extraction of coal at low temps. by a class of solvents with a generic structure, including Me₂NCOHME₂ [632-22-4] and (Me₂N)₃PO [680-31-9], was used to examine the nature of the extracted coal chems. The class of solvents with similar action, however, can be classified as **aprotic**, base solvents or, somewhat more broadly, specific solvents. The action of the solvents was then examined to postulate a mechanism of attack. Exptl. work conducted to explain the specific solvent attack included (1) pure solvent extraction, (2) extraction with mixts. with otherwise inert solvents and inhibitors, and (3) extraction with simultaneous catalytic enhancement attempts, including **water**-gas shift conversion. Thus, NMR and gas chromatog./mass spectroscopy of extract mols. and extraction with high-pressure CO in Me₂HCONMe₂ (containing 2% H₂O) was performed. The effects of solvent additives, such as cumene [98-82-8] and quinone [106-51-4], in large amts. of inert solvents, such as Tetralin [119-64-2], liminone [106908-29-6], or CS₂, on extraction were also determined

L20 ANSWER 19 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:439218 HCAPLUS
 DOCUMENT NUMBER: 105:39218
 TITLE: Coincident plasmids and antimicrobial resistance in marine bacteria isolated from polluted and unpolluted Atlantic Ocean samples
 AUTHOR(S): Baya, A. M.; Brayton, P. R.; Brown, V. L.; Grimes, D. J.; Russek-Cohen, E.; Colwell, R. R.
 CORPORATE SOURCE: Dep. Microbiol., Univ. Maryland, College Park, MD, 20742, USA
 SOURCE: Applied and Environmental Microbiology (1986), 51(6), 1285-92
 CODEN: AEMIDF; ISSN: 0099-2240
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Sewage effluent and outfall confluence samples were collected at the Barceloneta Regional Treatment Plant in Barceloneta, Puerto Rico; outfall confluence samples at Ocean City, Md., were also collected. Samples from uncontaminated open ocean areas served as clean-**water** controls. Bacteria were enriched in marine broth 2216 amended with 1 µg of one of a set of chemical selected for study per mL: nitrobenzene, di-Bu phthalate, m-cresol, o-cresol, 4-nitroaniline, bis(tributyltin) oxide, and quinone. Min. inhibitory concns. of the chemical were determined individually for all isolates. Bacterial isolates were evaluated for resistance to 9 different antibiotics and for the presence of plasmid DNA. Treated sewage contained

large nos. of bacteria simultaneously possessing antibiotic resistance, chemical resistance, and multiple bands of plasmid DNA. Bacteria resistant to penicillin, erythromycin, nalidixic acid, ampicillin, m-cresol, quinone, and bis(tributyltin) oxide were detected in nearly all samples, but only sewage outfall confluence samples yielded bacterial isolates that were resistant to streptomycin. Bacteria resistant to a combination of antibiotics, including kanamycin, chloramphenicol, gentamicin, and tetracycline, were isolated only from sewage effluent samples. Thus, bacterial isolates derived from toxic chemical wastes more frequently contain plasmid DNA and demonstrate antimicrobial resistance than do bacterial isolates from domestic sewage-impacted **waters** or from uncontaminated open ocean sites.

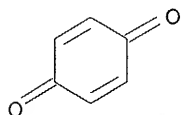
IT 106-51-4, biological studies

RL: BIOL (Biological study)

(plasmid-mediated resistance to, in marine **bacteria**,
water pollution in relation to)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 20 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:499810 HCAPLUS

DOCUMENT NUMBER: 103:99810

TITLE: Combined action of heavy metals and phenols on
aquatic organisms

AUTHOR(S): Gil, T. A.; Saksonov, M. N.; Stom, D. I.

CORPORATE SOURCE: NII Biol., Irkutsk, USSR

SOURCE: Vodnye Resursy (1985), (3), 118-21

CODEN: VDRSBK; ISSN: 0321-0596

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



I

AB In suspensions of *Beneckea harveyi* exposed to mixts. of HgCl₂ with p-benzoquinone (I) [106-51-4], resorcline [108-46-3] or hydroquinone [123-31-9] (5 min at 21°, pH 6.0), the fluorescence of the **bacteria** decreased in correlation with the concns. of both components. The decreases were additive, synergic, or antagonistic, depending on the concns. of the components. Thus, for the determination of maximum permissible concns. of **water** pollutants, it is not sufficient to consider only the concns. of each of the pollutants alone.

L20 ANSWER 21 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:424507 HCAPLUS

DOCUMENT NUMBER: 103:24507

TITLE: Hexanitrostilbene

INVENTOR(S): Duffin, Henry Charles; Golding, Peter;

Jaweera-Bandara, Asoka Manitha

PATENT ASSIGNEE(S): United Kingdom Secretary for Defence, UK
 SOURCE: Eur. Pat. Appl., 25 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 132990	A2	19850213	EP 1984-304895	19840718
EP 132990	A3	19850313		
EP 132990	B1	19870902		
R: DE, FR, GB, SE				
GB 2144736	A1	19850313	GB 1983-19850	19830722
US 4626606	A	19861202	US 1984-632294	19840719
			GB 1983-19850	A 19830722

PRIORITY APPLN. INFO.:

AB HNS [20062-22-0] is synthesized by oxidizing TNT [118-96-7] or 1,2-dipicrylethane (I) [5180-53-0] with free O, H₂O₂, or a benzoquinone in a medium containing an aprotic solvent, a protic solvent, and a basic alkali metal carboxylate. Thus, 0.64 g NaOBz [532-32-1] in 25 mL DMSO [67-68-5] was slowly added at 800 rpm to a solution of 1.9 g I in 25 mL DMSO at 25°. Dry air was pumped through the blue solution at .apprx.2 L/s until the color changed to red-brown (after .apprx.30 min), and the reaction was quenched by pouring into 100 mL **water** acidified with 1 mL concentrated HCl. The precipitate was isolated after standing for 10 min

and

dried at 60°. The yield of crude product was 0.96 g (96 mol%). Washing with MeOH and acetone to remove byproducts and DMSO gave 0.64 g (64 mol%) pure HNS. Solvent stripping of the acetone filtrate and drying gave 0.17 g (17 mol%) unreacted I. Conversion of I to other **water**-soluble byproducts was 0.15 g (15 mol%).

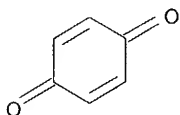
IT 106-51-4, uses and miscellaneous

RL: USES (Uses)

(oxidizing agents, in HNS synthesis from dipicrylethane and TNT in presence of **aprotic** and **protic** solvents and alkali metal carboxylate catalysts)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 22 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:137411 HCAPLUS

DOCUMENT NUMBER: 102:137411

TITLE: Removal of quinones from an aqueous environment by phenols and the effect of their mixing on the luminescence of the bacteria *Beneckea harveyi*

AUTHOR(S): Gil, T. A.; Nechaeva, V. I.; Balayan, A. E.; Shakhova, G. V.; Stom, D. I.; Koryakovtsev, A. A.

CORPORATE SOURCE: Irk. Gos. Univ., Irkutsk, USSR

SOURCE: Biologicheskije Nauki (Moscow) (1985), (1), 58-62

CODEN: BINKBT; ISSN: 0470-4606

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The addns. of monobasic phenols to **water** containing p-benzoquinone

(I) [106-51-4] decreased I concentration as determined by the potentiometric titration, polarog., and bioassay (luminescence of Benecka harvey bacteria and life span of Daphnia pulex). Thus, the addition of 10-2 M solution resorcinol [108-46-3] to an equal volume of 10-3 M I solution decreased I concentration by 78.5% in 30 min. This effect was due to I interactions with phenols leading to polyphenols of reduced bioactivity.

L20 ANSWER 23 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:73749 HCAPLUS

DOCUMENT NUMBER: 102:73749

TITLE: Glutathione S-transferase in **aquatic** macroinvertebrates and its interaction with different organic micropollutants

AUTHOR(S): Dierickx, Paul J.

CORPORATE SOURCE: Inst. Hyg. Epidemiol., Brussels, B-1050, Belg.

SOURCE: Science of the Total Environment (1984), 40, 93-102
CODEN: STENDL; ISSN: 0048-9697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The presence of GSH S-transferase (GST) [50812-37-8] in **aquatic** macroinvertebrates and its possible significance as a detoxification mechanism of organic micropollutants in the **aquatic** environment was investigated. GST was found in 20 macroinvertebrates (in adults as well as in **larvae**) and in insects as well as in other animal groups. The GST activities were relatively high, ranging from 10 to 600% of the activity found in rat liver. The interaction of quinones, o-chloranil [2435-53-2], and chlorophenoxyalkyl acids with the GST activity, in exts. from 3 different macroinvertebrates, revealed an inhibition which was quite similar to that previously found for rat liver GST. In Tubifex tubifex exts., at least 3 different GST isoenzymes could be demonstrated. These partially purified isoenzymes were used for the kinetic anal. of GST inhibition by 2,4-dichlorophenoxyalkyl acid and 1,4-benzoquinone [106-51-4], using Lineweaver-Burk plots. The same kinetic patterns were observed as for rat liver GST. Interactions of the compds. investigated with **aquatic** macroinvertebrate and with rat liver GST were in very good agreement. Thus, macroinvertebrate GST may play a key role in the detoxification of organic micropollutants in the **aquatic** environment.

L20 ANSWER 24 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:60757 HCAPLUS

DOCUMENT NUMBER: 102:60757

TITLE: Oxygen supply to immobilized cells. 4. Use of p-benzoquinone as an oxygen substitute

AUTHOR(S): Adlercreutz, Patrick; Mattiasson, Bo

CORPORATE SOURCE: Chem. Cent., Univ. Lund, Lund, S-220 07, Swed.

SOURCE: Applied Microbiology and Biotechnology (1984), 20(5), 296-302
CODEN: AMBIDG; ISSN: 0175-7598

DOCUMENT TYPE: Journal

LANGUAGE: English

AB O2 supply is a critical point in tech. processes when aerobic cells are used in immobilized preps. In this study, p-benzoquinone [106-51-4] is used as a substituent for O2 in the oxidation of glycerol [56-81-5] to dihydroxyacetone [96-26-4] by immobilized **Gluconobacter** oxydans cells. The reaction rate was much higher when p-benzoquinone was used compared to when O2 was used. In an experiment with free cells, p-benzoquinone gave a rate >4-fold that of O2, and with immobilized cells, the difference was even greater. p-Benzoquinone is more effective than O2, because it gives a higher maximal reaction rate (the reason for this fact is discussed) and because it is more soluble in **water** than O2. The operational stability of the process is comparatively good. In 1 experiment,

the productivity decreased from 60 to 10 mmol/h-g over an 8-day period when p-benzoquinone was used. When O₂ was used in a similar experiment, the productivity decreased from 14 to 6 mmol/h-g. The byproduct formed from p-benzoquinone, hydroquinone, can be oxidized to p-benzoquinone, which can be reused. Seven successive regenerations of p-benzoquinone were performed without any loss of efficiency.

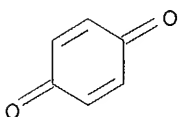
IT 106-51-4, biological studies

RL: BIOL (Biological study)

(as oxygen substitute, in glycerol oxidation to dihydroxyacetone by immobilized *Gluconobacter oxydans*)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 25 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:494445 HCAPLUS

DOCUMENT NUMBER: 101:94445

TITLE: Photoproduction of hydrogen using plant and microbial membrane systems. Final subcontract report

AUTHOR(S): Olson, J. M.

CORPORATE SOURCE: Brookhaven Natl. Lab., Upton, NY, USA

SOURCE: Report (1983), SERI/STR-231-1874; Order No.

DE84000062, 35 pp. Avail.: NTIS

From: Energy Res. Abstr. 1984, 9(9), Abstr. No. 16095

DOCUMENT TYPE: Report

LANGUAGE: English

AB A solar H generator was assembled from unit-membrane vesicles from green photosynthetic **bacteria**. The vesicles contain light-harvesting **bacteriochlorophyll a** [17499-98-8], photochem. reaction centers, and various electron carriers that deliver electrons from ascorbic acid [50-81-7] to exogenous ferredoxin and hydrogenase [9027-05-8]. H is formed with an overall quantum requirement of .apprx.10 photons/electron transferred. Of 21 polypeptides found in the vesicle membranes 5 (25.0, 25.5, 38.5, 69, and 93 kD) have the possibility of a specific association with the reaction center. Another type of photosynthetic membrane from a thermophilic **cyanobacterium** contains both photosystem I and photosystem II reaction centers. Photosystem II particles prepared with lauryl dimethylamine oxide [1643-20-5] evolve O from H₂O and deliver electrons to a weak reductant, dimethylbenzoquinone [30998-92-6], with an overall quantum requirement of .apprx.5 photons/electron. If vesicles from green **bacteria** can be coupled to membranes or photosystem II particles from **cyanobacteria**, the combined system in sunlight should generate H from H₂O with a maximum energy conversion efficiency of .apprx.10%.

L20 ANSWER 26 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:97724 HCAPLUS

DOCUMENT NUMBER: 100:97724

TITLE: Quenching the luminescence of luminescent bacteria as a test for estimating the toxicity of phenol components of sewage

AUTHOR(S): Gil, T. A.; Balayan, A. E.; Stom, D. I.

CORPORATE SOURCE: USSR

SOURCE: Mikrobiologiya (1983), 52(6), 1014-16

CODEN: MIKBA5; ISSN: 0026-3656

DOCUMENT TYPE: Journal
 LANGUAGE: Russian

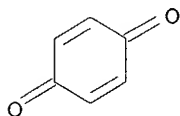
AB Among the 3 tests used for studying the toxicity of wastewater phenols to luminescent **bacteria** (*Beneckea harvey*), quenching of the luminescence was most sensitive indicator compared to inhibition of dehydrogenase [9035-82-9] activity and **bacterial** multiplication. The luminescence quenching was a rapid test with a response time of 10 s, whereas the dehydrogenase and multiplication tests required 6 h and 1 day, resp. The phenols studied could be placed in the decreasing toxicity order (all tests): p-benzoquinone [106-51-4], hydroquinone [123-31-9], resorcinol [108-46-3], PhOH [108-95-2]. The quenching of the **bacterial** luminescence, seen under the effect of the toxicants, can also be observed visually (instead of luminometer used in the actual test); however, the toxicity and accuracy are reduced.

IT 106-51-4, biological studies

RL: BIOL (Biological study)
 (luminescence quenching by, of **bacteria**, toxicity in relation to)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 27 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:609949 HCAPLUS

DOCUMENT NUMBER: 97:209949

TITLE: Four-hour algal bioassays for assessing the toxicity of coal-derived materials

AUTHOR(S): Giddings, J. M.

CORPORATE SOURCE: Environ. Sci. Div., Oak Ridge Natl. Lab., Oak Ridge, TN, 37830, USA

SOURCE: U. S. Environ. Prot. Agency, Off. Res. Dev., [Rep.] EPA (1981), EPA-600/9-81-018, Proc. Symp. Process Meas. Environ. Assess., 2nd, 104-16
 CODEN: XPARD6; ISSN: 0092-8054

DOCUMENT TYPE: Report

LANGUAGE: English

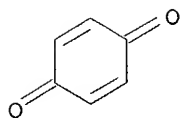
AB Algal cultures or natural algal communities are exposed to coal-derived materials for 4 h. Photosynthesis is determined by the ¹⁴C-bicarbonate method during the final 2 h of exposure and compared with controls for a measure of toxicity. In bioassays with individual aromatic compds., quinones, and aromatic amines were particularly toxic to algae; azaarenes, and thiophenes were the least toxic classes tested. Expts. with the **water**-soluble fractions (WSFs) of >20 natural and synthetic oils showed that coal liquefaction products are considerably more toxic than petroleum products; shale oils are intermediate in toxicity. Further studies with particular subfractions of several SWFs have identified ether-soluble bases as the major contributors to the toxicity of coal-derived oils. The 4-h photosynthesis test has several advantages over the Algal Assay Bottle Test for measuring the toxicity of complex materials.

IT 106-51-4, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (toxicity of, to **algae**)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 28 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:449310 HCAPLUS

DOCUMENT NUMBER: 97:49310

TITLE: A comparison of log P and molecular connectivity in the structure-activity analysis of some antimicrobial agents

AUTHOR(S): Boyd, J. C.; Millership, J. S.; Woolfson, A. D.

CORPORATE SOURCE: Dep. Pharm., Queen's Univ. Belfast, Belfast, BT9 7BL, UK

SOURCE: Journal of Pharmacy and Pharmacology (1982), 34(3), 158-61

CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Several congeneric series of antimicrobial agents were investigated using mol. connectivity as the descriptor of mol. structure. The fungicidal activity of p-hydroxybenzoates, aliphatic carboxylic acids, benzyl isothiocyanates, and quinones and the antibacterial activity of alkyl β-naphthols and benzyl alcs. were tested. In all cases, mol. connectivity gave comparable or improved correlations with biol. activity compared with the logarithm of the octanol-water coefficient of the mol. (log P). Thus, the use of computer-generated connectivity terms has advantages over the calculated log P values in its ease of application and should be considered at least for initial screening of structure-activity data.

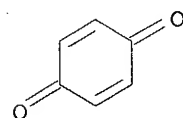
IT 106-51-4, biological studies 137-18-8 553-97-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(fungicidal activity of, structure in relation to)

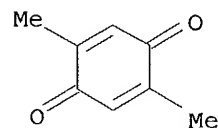
RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



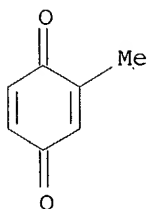
RN 137-18-8 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dimethyl- (9CI) (CA INDEX NAME)



RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



L20 ANSWER 29 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:175979 HCAPLUS

DOCUMENT NUMBER: 96:175979

TITLE: On improvement of garlic productivity by inactivation of virus in garlicks

AUTHOR(S): Lee, Chang Un

CORPORATE SOURCE: Coll. Agric. Anim. Sci., Yeungnam Univ., Gyeongsan, 632, S. Korea

SOURCE: Han'guk Sikmul Poho Hakhoechi (1981), 20(1), 6-14
CODEN: HSHCA8; ISSN: 0367-6285

DOCUMENT TYPE: Journal

LANGUAGE: Korean

AB The effect of heat or chemotherapeutic treatment on the mosaic virus-infected garlic (*Allium sativum*) scales and that of chemotherapeutic agents added to the culture medium were studied. The treatment of the virus-infected garlic scales at 37.apprx.57% for 35 days to 1 h in water or in air showed no effect on inactivating the virus. Although treatment of the garlic scales at 62.apprx.72° for 90 to 5 min reduced the mosaic symptom of the leaves of the plants grown after the heat treatment, it reduced the growth vigor so greatly that complete inactivation of the virus in garlicks was not feasible. The mosaic symptom on the leaves was reduced when the infected garlic scales were grown after 24 h soaking in 10.apprx.50 ppm Malachite Green [569-64-2], 2,4-D [94-75-7], or in 20.apprx.100 ppm Quinhydrone [106-34-3]. These agents, however, inhibited the growth of garlic plant at the high concentration. Garlic scales soaked in 10.apprx.50 ppm NAA [86-87-3] showed the least mosaic symptom. When incorporated into the modified Murashige-Skoog's medium, 0.5.apprx.1.5 ppm NAA could inactivate the mosaic virus in newly-developed garlic plants showing no mosaic symptom on the leaves, no inclusion bodies and intact nuclei in the leaf tissue cells.

IT 106-34-3

RL: BIOL (Biological study)
(mosaic virus control by, in garlic, phytotoxicity in relation to)

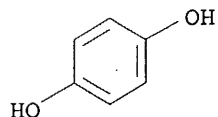
RN 106-34-3 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, compd. with 1,4-benzenediol (1:1) (9CI) (CA INDEX NAME)

CM 1

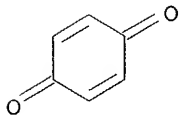
CRN 123-31-9

CMF C6 H6 O2



CM 2

CRN 106-51-4
CMF C6 H4 O2



L20 ANSWER 30 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:117107 HCAPLUS

DOCUMENT NUMBER: 96:117107

TITLE: Comparison of bacterial luminescence and fish bioassay results for fossil-fuel process **waters** and phenolic constituents

AUTHOR(S): Lebsack, M. E.; Anderson, A. D.; DeGraeve, G. M.; Bergman, H. L.

CORPORATE SOURCE: Alcohol. Res. Treat. Cent., VA Hosp., Bronx, NY, 10468, USA

SOURCE: ASTM Special Technical Publication (1981), 737 (Aquat. Toxicol. Hazard Assess.), 348-56
CODEN: ASTTA8; ISSN: 0066-0558

DOCUMENT TYPE: Journal

LANGUAGE: English

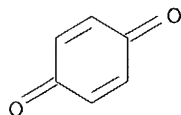
AB EC50 values (50% luminescence inhibition concentration) using Photobacterium fischeri (P. phosphoreum) and LC50 (median lethal concentration) for rainbow trout and fathead minnow were similar. For the fossil fuel process **waters** the luminescence EC50 values were usually within a factor 2 of the fish LC50 values (Paraho 77-78 being a notable exception). A comparison of the bacterial and fish results for phenolic compds. indicates somewhat more variability, but the general toxicity trends are similar. Overall, for all the process **waters** and phenolic compds., the fish toxicity tests were more sensitive in about half of the cases. This type of toxicity testing system has potential value for semicontinuous monitoring of industrial or municipal effluents.

IT 106-51-4, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, **bacterial** luminescence assay for evaluation of, fish assay in comparison with)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



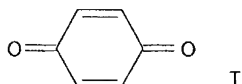
L20 ANSWER 31 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:42246 HCAPLUS

DOCUMENT NUMBER: 94:42246

TITLE: Evaluation of the mutagenic and toxic action of pulp and paper production wastewater and components on Drosophila

AUTHOR(S): Grechanyi, G. V.; Zasukhina, O. V.; Nikitin, A. Ya.
 CORPORATE SOURCE: USSR
 SOURCE: Issled. Biol. Deistviya Antropogennykh Faktorov, Zagryaz. Vodoemy (1979), 57-69. Editor(s): Kozhova, O. M. Irkutskii Univ.: Irkutsk, USSR.
 CODEN: 44QKAM
 DOCUMENT TYPE: Conference
 LANGUAGE: Russian
 GI



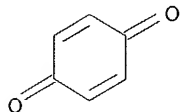
AB Biol. treatment of effluents from the Baikal Paper and Cellulose Combine in an aeration pond greatly increased their embryotoxicity to 1 D. melanogaster strain and induced toxicity to another strain which tolerated untreated black and white water, and chemical treated combined effluent. Larvae were raised on a yeast medium spiked with 0.012-1.2 g effluents/L. Replacing wastewaters by 0.012-1.2 g p-quinone (I) [106-51-4] increased the mortality of eggs sired by males raised on I-amended medium. The effluents and I showed no direct toxicity to larvae reared on them. Rearing the less susceptible strain chronically on I eliminated it within 17 generations, whereas the strain more susceptible in the 1st generation survived longer.

L20 ANSWER 32 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:631936 HCAPLUS
 DOCUMENT NUMBER: 93:231936
 TITLE: Acute and embryo-larval toxicity of phenolic compounds to aquatic biota
 AUTHOR(S): DeGraeve, G. M.; Geiger, D. L.; Meyer, J. S.; Bergman, H. L.
 CORPORATE SOURCE: Dep. Zool. Physiol., Univ. Wyoming, Laramie, WY, 82071, USA
 SOURCE: Archives of Environmental Contamination and Toxicology (1980), 9(5), 557-68
 CODEN: AECTCV; ISSN: 0090-4341
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Because of the prevalence of phenolic compds. in various types of effluents, both acute and embryo-larval bioassays were performed on 8 phenolic compds. with rainbow trout (Salmo gairdneri), fathead minnows (Pimephales promelas), and Daphnia pulicaria. In flow-through bioassays, the 96-h median lethal concentration (LC50) values for rainbow trout and fathead minnows ranged from <0.1 mg/L for hydroquinone [123-31-9] to >100 mg/L for resorcinol [108-46-3]. D. pulicaria was consistently the least sensitive species tested as measured in 48-h bioassays, while fathead minnows and rainbow trout varied in their relative sensitivity to phenolics as measured in 96-h tests. Fathead minnows were more sensitive to phenol [108-95-2] at 25° than at 14°. In embryo-larval bioassays with phenol, fathead minnow growth was significantly decreased by 2.5 mg/L, while rainbow trout growth was significantly decreased by 0.20 mg/L. For both species, the embryo-larval effects concentration was 1.1% of the 96-h LC50. Another embryo-larval bioassay was attempted with p-benzoquinone [106-51-4], a highly toxic phenolic compound found in fossil fuel processing wastewaters, which was discontinued because the compound was rapidly degraded chemical or biol. in the headtank and aquaria.

IT 106-51-4, biological studies
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (toxicity of, to **aquatic biota**)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 33 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1980:562090 HCAPLUS
 DOCUMENT NUMBER: 93:162090
 TITLE: The disposition of aromatic hydrocarbons in adult spot shrimp (*Pandalus platyceros*) and the formation of metabolites of naphthalene in adult and larval spot shrimp
 AUTHOR(S): Sanborn, H. R.; Malins, D. C.
 CORPORATE SOURCE: Northwest Alaska Fish. Cent., NOAA, Seattle, WA, 98112, USA
 SOURCE: Xenobiotica (1980), 10(3), 193-200
 CODEN: XENOBH; ISSN: 0049-8254
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Adult spot shrimp exposed to 110 ppb of the **water**-soluble fraction of Prudhoe Bay crude oil for 1 wk accumulated a variety of low-mol.-weight aromatic hydrocarbons (primarily C1-C5 substituted derivs.) in thoracic and abdominal tissues. In adult shrimps exposed to 14C- and 3H-labeled naphthalene [91-20-3] in seawater, nonconjugated derivs. (quinone [106-51-4], α -naphthol [90-15-3], and naphthalene-1,2-dihydrodiol [7234-04-0]) represented 69% of the total conversion products, conjugated metabolites (sulfate, glucuronide, and glycoside) each accounted for $\leq 7\%$, and an unidentified metabolite accounted for 16% of the total conversion products. **Larval** shrimps exposed to naphthalene showed different compns.; naphthyl sulfate [69206-01-5] and naphthol represented 39 and 44%, resp., of the total conversion products and quinone and dihydrodiol represented small percents (7 and 4%, resp.).

L20 ANSWER 34 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1980:401667 HCAPLUS
 DOCUMENT NUMBER: 93:1667
 TITLE: Effect of phenols of wastewaters on some energy-dependent parameters of Chaveal alga cells
 AUTHOR(S): Plekhanov, S. E.; Stom, D. I.; Khitrov, Yu. A.; Yasinovskii, V. G.
 CORPORATE SOURCE: Mosk. Gos. Univ., Moscow, USSR
 SOURCE: Biologicheskie Nauki (Moscow) (1980), (2), 40-3
 CODEN: BINKBT; ISSN: 0303-4119
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

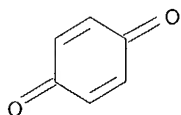


I

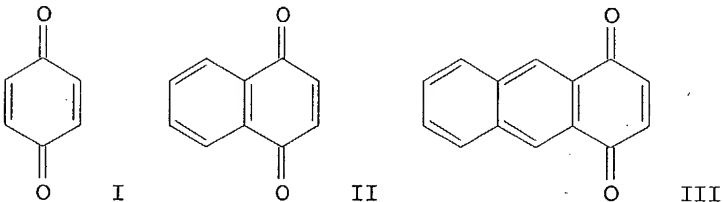
AB The effects of PhOH [108-95-2], hydroquinone (I) [123-31-9], p-benzoquinone [106-51-4], resorcinol [108-46-3], pyrocatechol [120-80-9], and guaicol [90-05-1] was examined on the isolated internodal cells of *Nitella* growing in wastewater (during various stages of purification). The phenols inhibited the rate of cytoplasmic movement. At $1 + 10^{-3}$ and $5 + 10^{-4}M$, they reduced the elec. p.d. at the plasmalemma and increased the elec. resistance. A further increase in the concentration of the phenols caused an irreversible decrease in these changes and finally cell death. Changes in the p.d. and elec. resistance, shown by the plasmalemma at low concns. of phenols, may be useful criteria to evaluate the toxicity of phenols.

IT 106-51-4, biological studies
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (toxicity of, to algae, elec. activity in relation to)

RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 35 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1980:16515 HCAPLUS
 DOCUMENT NUMBER: 92:16515
 TITLE: Acute toxicity to *Selenastrum capricornutum* of aromatic compounds from coal conversion
 AUTHOR(S): Giddings, Jeffrey M.
 CORPORATE SOURCE: Environ. Sci. Div., Oak Ridge Natl. Lab., Oak Ridge, TN, 37830, USA
 SOURCE: Bulletin of Environmental Contamination and Toxicology (1979), 23(3), 360-4
 CODEN: BECTA6; ISSN: 0007-4861
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB In freshwater alga (*S. capricornutum*) exposed to coal-derived aromatic compds. at concns. of 10, 100 and 1000 mg/L (soluble compds.) or at 1, 10 and 100% saturation (compds. whose solubility was <1000 mg/L), p-benzoquinone (I) [106-51-4] and 1,4-naphthoquinone (II) [130-15-4] were the most toxic compds., based on short-term photosynthetic inhibition as the measure of toxic response. 1,4-Anthraquinone (III) [635-12-1] was essentially nontoxic to the algae, as were all the other 3-ring

compds. except acridine [260-94-6]. Aromatic amines (aniline [62-53-3] and 1-naphthylamine [134-32-7]) were highly toxic as was 2-naphthol [135-19-3]. Thiophenes and azaarenes were only slightly toxic except at the highest concns. The other classes of aromatic compds. (methylated aroms. and hydrocarbons) were intermediate in toxicity. In all cases, 2-ring compds. were more toxic than related 1-ring compds.

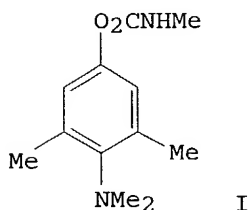
L20 ANSWER 36 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:165148 HCAPLUS
DOCUMENT NUMBER: 88:165148
TITLE: Possible mechanism of action of quinone pesticides on the protoplasmic streaming in marine plants
AUTHOR(S): Stom, D. I.; Rogozina, N. A.
CORPORATE SOURCE: Biol.-Geogr. Nauchno-Issled. Inst., Irkutsk, USSR
SOURCE: Eksperimental'naya Vodnaya Toksikologiya (1976), 6, 111-18
CODEN: EKVTA6; ISSN: 0367-0724
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Cessation of protoplasmic streaming in *Nitella* and *Elodea canadensis* was an earlier indicator of damage from phenols (such as hydroquinone [123-31-9] and resorcinol [108-46-3]) and quinones (including p-benzoquinone [106-51-4] and β -naphthoquinone [524-42-5]) than was plasmolysis and deplasmolysis. The quinones and phenols oxidizable to quinones also inhibited ATPase [9000-83-3] activity. A possible mechanism for the damaging effect of quinone pesticides on protoplasm streaming is blocking of the -SH groups and inactivation of the thiol enzymes, especially ATPase.

L20 ANSWER 37 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:70423 HCAPLUS
DOCUMENT NUMBER: 88:70423
TITLE: A new degradation product of the insecticide mexacarbate found in fresh water
AUTHOR(S): Roberts, Richard B.; Look, Melvin; Haddon, William F.; Dickerson, Thomas C.
CORPORATE SOURCE: Pac. Southwest Forest Range Exp. Stn., Forest Serv., Berkeley, CA, USA
SOURCE: Journal of Agricultural and Food Chemistry (1978), 26(1), 55-9
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The carbamate insecticide mexacarbate (I) [315-18-4] was degraded in plants and animals by oxidation of the dimethylamino group and by hydrolysis of the carbamate moiety. In water solns. of different pH

values, essentially the same degradation products were found:
 4-methylamino-3,5-xylyl methylcarbamate [10389-50-1], 4-amino-3,5-xylyl methylcarbamate [831-76-5], 4-methylformamido-3,5-xylyl methylcarbamate [10233-94-0], 4-formamido-3,5-xylyl methylcarbamate [10233-95-1], and 4-dimethylamino-3,5-xylyl hydroxymethylcarbamate [10310-18-6].
 Additional products identified included 4-dimethylamino-3,5-xyleneol [6120-10-1] and 2-hydroxy-3,5-dimethyl-p-benzoquinone [2913-40-8], a new degradation product. Bioassay of this new degradation product on sixth stage western spruce **budworm** (*Choristoneura occidentalis*) **larvae** indicated little or no toxicity at the rate of 0.1 mg/g by topical application and 0.05 mg/g by injection.

L20 ANSWER 38 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:588993 HCAPLUS

DOCUMENT NUMBER: 85:188993

TITLE: Study of the photoreduction of exogeneous electron acceptors by blue-green algae. Mediator mechanism of electron transport through a biomembrane

AUTHOR(S): Varfolomeev, S. D.; Zaitsev, S. V.; Belogurova, N. G.; Berezin, I. V.; Nikitina, K. A.; Gusev, M. V.

CORPORATE SOURCE: Chem. Dep., M. V. Lomonosov State Univ., Moscow, USSR

SOURCE: Bioorganicheskaya Khimiya (1976), 2(10), 1395-403

CODEN: BIKHD7; ISSN: 0132-3423

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB In the blue-green algae *Anabaena variabilis* and *Anacystis nidulans*, the photoredn. of K ferricyanide took place only in the presence of p-benzoquinone. The photoredn. reaction is inhibited by 3-(3,4-dichlorophenyl-1,1-dimethylurea), this fact being indicative of the **water** splitting system participation in the process. A mechanism is suggested to account for p-benzoquinone effects, which involves the stages of photoredn. of p-benzoquinone and electron transport through a biomembrane onto K ferricyanide.

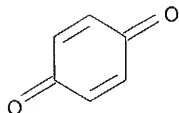
IT 106-51-4, biological studies

RL: BIOL (Biological study)

(in photoredn. of potassium ferricyanide with blue-green algae)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 39 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1966:22699 HCAPLUS

DOCUMENT NUMBER: 64:22699

ORIGINAL REFERENCE NO.: 64:4201g-h,4202a-b

TITLE: Fungicides containing di-, tri-, and tetramethyl-1,4-benzoquinone monooxime and **water**-soluble salts thereof

PATENT ASSIGNEE(S): United States Rubber Co.

SOURCE: 9 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6413711		19650701	NL	
PRIORITY APPLN. INFO.:			US	19631230

AB The fungicides are especially suitable to apply to the soil to protect seeds and sprouting plants against especially *Rhizoctonia solani*, using preferably 0.28-5.6 kg./ha. on seed rows of a width of 5 cm. and a depth of 5 cm. and 1 m. apart, or using 11.2-224 kg./ha. when spraying on all of the soil. A powdered composition for spraying consists, e.g., of 2,5-dimethyl-1,4-benzoquinone monooxime (I) 75, Dixie Clay (kaolin) 12, Polyfon H (Na lignosulfonate) 2, Triton X-120 5, and ethylene glycol 6 parts, and preferably 0.1-3 parts powdered carrier as clay or mineral silicates per part active ingredient. In testing the fungicidal activity in cotton plants, 66 mg. was mixed with 450 g. sand. The premixt. was mixed with 28.5 kg. earth to obtain a concentration of 20 ppm. The mixture was put in pots (diameter 10 cm.), after which

5

cotton seeds "Fox-4" were put on the soil. A grain of oats infected with *R. solani* of a culture 2 weeks old, was put between the cotton seeds in 5 pots. In comparison 5 seeds were put in 5 pots containing untreated earth without the infected grain of oats and the same with the infected grain of oats. The seeds were covered with a 1.25-cm. layer of earth. The pots were kept at 22-6° in a moist atmospheric After 2 and 3 weeks the percent of surviving plants based on sprouted plants was determined Results are given in the table. %, sprouted, plants, %, surviving, plants; I 20 ppm., 80, 76; 2,6-dimethyl-1,4-benzoquinone monooxime 20 ppm., 84, 76; untreated infected earth, 76, 0; untreated noninfected earth, 92, 92; 2,3,5-trimethyl-1,4-benzoquinone monooxime 20 ppm., 72, 68; 2,3,5,6-tetramethyl-1,4-benzoquinone monooxime 80, , ; ppm., 80, 76; untreated infected earth, 42, 0; untreated noninfected earth, 88, 88; I 20 ppm. + tetramethylthiuram disulfide (II) 20, , ; ppm., 82, 93; I 10 ppm. + II 20 ppm., 82, 66; untreated infected earth, 86, 7; untreated noninfected earth, 84, 98;

IT 30554-01-9, p-Benzoquinone, 2,6-dimethyl-, oxime
(as fungicide)

RN 30554-01-9 HCAPLUS

CN p-Benzoquinone, 2,6-dimethyl-, monooxime (8CI) (CA INDEX NAME)

CM 1

CRN 7803-49-8

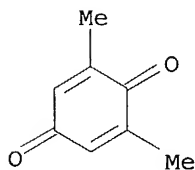
CMF H3 N O

H₂N-OH

CM 2

CRN 527-61-7

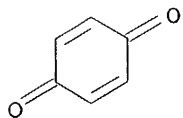
CMF C8 H8 O2



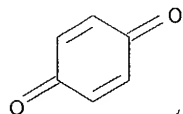
IT 106-51-4, p-Benzoquinone

(derivs., as fungicides)

RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 40 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1957:57399 HCAPLUS
 DOCUMENT NUMBER: 51:57399
 ORIGINAL REFERENCE NO.: 51:10663d-e
 TITLE: Pristimerin III. Antibacterial activity of some simple orthoquinones
 AUTHOR(S): Kamat, V. N.; de Sa, J.; Fernandes, F.; Bhatnagar, S. S.
 CORPORATE SOURCE: St. Xavier's Coll., Bombay
 SOURCE: J. Sci. Ind. Research (India) (1956), 15C, 8-9
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Only the o-quinones were active against organisms of the viridans group. An increase in the **water** solubility of quinones and in the number of rings present in the mol. decreases activity. 1,2-Benzoquinone, 1,2-naphthoquinone, 4-amino-1,2-naphthoquinone, and 9,10-phenanthraquinone (I) show 2.5-12.5 times the activity of pristimerin (II) against Micrococcus pyogenes var. aureus, (III), Diplococcus pneumoniae, type II, Streptococcus pyogenes, and S. viridans I with the exception that I is equal but not superior to II in its activity against III.
 IT 106-51-4, p-Benzoquinone
 (effect on **bacterial** growth)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



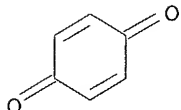
L20 ANSWER 41 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1948:4697 HCAPLUS
 DOCUMENT NUMBER: 42:4697
 ORIGINAL REFERENCE NO.: 42:1014e-f
 TITLE: Derivatives of halogenated quinones as fungicides
 INVENTOR(S): Ladd, Elbert C.; Harvey, Merlin P.
 PATENT ASSIGNEE(S): U.S. Rubber Co.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2430722		19471111	US	

AB Derivs. of tetrachloro-(I) and tetrabromo-p-quinone and of 2,3-dichloro- and 2,3-dibromo-1,4-naphthoquinone, obtained by replacement of one of the

halogens by the residue obtained by removing a H from a compound containing an active -CH₂-, are fungicides. Thus the diethyl ester of 3,5,6-trichloro-1,4-benzoquinone-2-oxalacetic acid, m. 102-3.5°, from EtOH was prepared, by addition of 3 mols. of (CH₃COONa)(CO₂Et)₂ to 1 mol. I in acetone. After 1.5 hrs., the solution was filtered, acidified with HCl, diluted with water, and the solid recrystd. Cf. C.A. 39, 1246.4; 41, 5899h, 5900a.

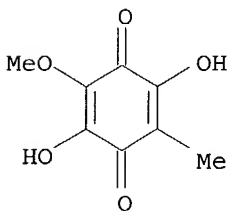
IT 106-51-4, p-Benzoquinone
(derivs., for fungicides)
RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 42 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1947:31250 HCAPLUS
DOCUMENT NUMBER: 41:31250
ORIGINAL REFERENCE NO.: 41:6302a-c
TITLE: Routine examination for antibiotics produced by molds
AUTHOR(S): Heatley, N. G.; Philpot, Flora J.
CORPORATE SOURCE: Univ. of Oxford
SOURCE: Journal of General Microbiology (1947), 1, 232-7
CODEN: JGMIAN; ISSN: 0022-1287
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

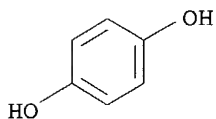
AB Routine performance of a few simple tests on culture filtrates of antibiotic-producing fungi serves to identify presumptively the presence of any of the following 14 antibiotics; penicillin, helvolic acid, mycophenolic acid, proactinomycin, citrinin, gliotoxin, puberulic acid, fumagatin, spinulosin, patulin (clavacin), aspergillic acid, penicillic acid, kojic acid and streptomycin. The tests are: stability at pH 2.0 and 9.5; ether-water partition at pH 2.0, 6.0-7.0 and 9.0; relative activities towards specified strains of Staphylococcus aureus and Escherichia coli, destruction by penicillinase, color reactions and volatility with steam. In some cases it may be essential to isolate the inhibitor and characterize it by the usual chemical criteria.

IT 85-23-4, Spinulosin
(from molds)
RN 85-23-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3-methoxy-6-methyl- (9CI) (CA INDEX NAME)

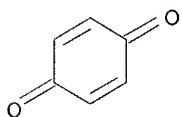


L20 ANSWER 43 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1946:37655 HCAPLUS

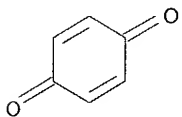
DOCUMENT NUMBER: 40:37655
 ORIGINAL REFERENCE NO.: 40:7277c-d
 TITLE: The antibiotic action in vitro of naphthoquinone and of synthetic **water**-soluble vitamin K against staphylococcus, B. diphtheriae, and B. typhi
 AUTHOR(S): Nassi, Lelio
 CORPORATE SOURCE: Univ. Florence, Italy
 SOURCE: Bollettino - Societa Italiana di Biologia Sperimentale (1946), 21, 141-4
 CODEN: BSIBAC; ISSN: 0037-8771
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Naphthoquinone (0.04%) and 2-methyl-1,4-disuccinylnaphthoquinone (0.1%) show antibiotic activity, particularly against staphylococcus.
 IT 106-34-3, Quinhydrone 106-51-4, Quinone (bactericidal action of)
 RN 106-34-3 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, compd. with 1,4-benzenediol (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 123-31-9
 CMF C6 H6 O2



CM 2
 CRN 106-51-4
 CMF C6 H4 O2



RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

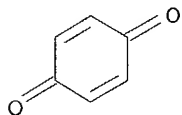


L20 ANSWER 44 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1919:8838 HCAPLUS
 DOCUMENT NUMBER: 13:8838
 ORIGINAL REFERENCE NO.: 13:1718f-i
 TITLE: Some factors influencing the effect of dyes and allied compounds on bacteria

AUTHOR(S): Graham-Smith, G. S.
 SOURCE: Journal of Hygiene (1919), 18, 1-32
 CODEN: JOHYAY; ISSN: 0022-1724
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB In cultures the effects of homoflavine and quinone, the compds. most thoroughly investigated, vary on each species of organism with each change of composition of the medium, whether the change is brought about by altering the proportion of any constituent, or by adding new constituents, and also with variations in the number and age of the organism. In each medium the concentration of the compound which inhibits each species differs, and it is probable that still other concns. are required when mixed cultures are used, though this is not established by experiment. In wounds the conditions are more complex than in cultures. The conditions in no two wounds are likely to be identical, and are constantly altering, in chemical composition, number of species, and interrelationships of organisms. S. concludes as follows: A wound must be thoroughly cleansed before the application of the dye since the complex organic fluids present may interfere with the action of the solution. The compound should be dissolved in a fluid with the optimum reaction for that substance if such a reaction is not harmful to the tissues. Some compds. are more efficient than others against certain species of bacteria. Compds. are more effective in the early stages of an infection since the organisms later increase in number, become accustomed to their surroundings, and are protected in the fluids. It would be desirable to test the action on wounds of a solution in distilled water of 1:10000 hemoflavine, 1:10000 quinone, 1:100000 crystal violet. Some good results have been obtained in pyorrhea, stomatitis, and gingivitis. Plates and references are given.

IT 106-51-4, Quinone
 (effect on bacteria)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



=> □

=> d stat que nos

L7 STR
 L9 SCR 1839
 L11 4180 SEA FILE=REGISTRY SSS FUL L7 NOT L9
 L14 STR
 L15 901 SEA FILE=REGISTRY SUB=L11 SSS FUL L14
 L16 16802 SEA FILE=HCAPLUS ABB=ON PLU=ON L15
 L18 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L) (?PORIFER? OR ?HELMINTH?
 OR ?COELOMA? OR ?ANNELID? OR ?WORM? OR ?MOLLUSK? OR ?BIVAL?
 OR ?LARV? OR ?COPEPOD? OR ?OSTRACOD? OR ?MYSID? OR ?GAMMARID?
 OR ?DECAPOD? OR ?TELEOS? OR ?STARFISH?)
 L19 361 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L) (PEST? OR AQUACID? OR
 ?VIRUS? OR ?PROTI? OR ?FUNGI? OR MOLD OR MOLDS OR ANTIMOLD OR
 ?PLANKTON? OR ?DEMERS? OR ?BENTHI? OR ?BIOTA? OR ?BACTER? OR
 ?PROTOZO? OR ?ALGAE? OR ?PYRROP? OR ?CRYPTOP? OR ?CHRYSOPH?)
 L20 44 SEA FILE=HCAPLUS ABB=ON PLU=ON (L18 OR L19) AND (WATER OR
 AQUA?)
 L21 3 SEA FILE=HCAPLUS ABB=ON PLU=ON ((L18 OR L19) AND (MARIN? OR

SEAWATER)) NOT L20

=>
=>

=> d ibib abs hitstr l21 1-3

L21 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:568535 HCAPLUS

DOCUMENT NUMBER: 141:84034

TITLE: Bactericides for **marine** periphytic bacteria
containing natural products, and method and agent for
controlling bioadhesion of **marine** organisms
to ship bottomINVENTOR(S): Ishii, Akira; Kohiyori, Hideki; Makita, Yoji; Umeno,
Aya; Oi, KentaPATENT ASSIGNEE(S): National Institute of Advanced Industrial Science and
Technology, JapanSOURCE: Jpn. Kokai Tokyo Koho, 7 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004196677	A2	20040715	JP 2002-364508	20021217
PRIORITY APPLN. INFO.:			JP 2002-364508	20021217

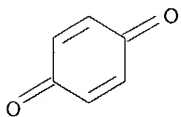
AB The bactericides, which control **marine** periphytic bacteria, thus
preventing biofouling of barnacle larvae, etc., contain ≥ 1 selected
from organism exts., spices, polysaccharides, organic acids, and proteins.
Adhesion of **marine** organisms is prevented by coating ship
bottoms with paints containing ≥ 1 of the above components optionally
adsorbed by carriers. Thus, hinokitiol (I) inhibited growth of
Pseudoalteromonas carrageenovora. Antifouling effect of a paint containing I
on a ship bottom was also shown.

IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies
RL: BSU (Biological study, unclassified); BUU (Biological use,
unclassified); TEM (Technical or engineered material use); BIOL
(Biological study); USES (Uses)

(bactericides for **marine** periphytic
bacteria containing organism exts., spices, polysaccharides, organic
acids, or proteins, and their use for ship bottom antifouling paints)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L21 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:561826 HCAPLUS

DOCUMENT NUMBER: 122:287292

TITLE: Inhibitory effect of bacterial ubiquinones on the
settling of barnacle, *Balanus amphitrite*

AUTHOR(S): Kon-ya, K.; Shimidzu, N.; Otaki, N.; Yokoyama, A.;

CORPORATE SOURCE: Adachi, K.; Miki, W.
Shimizu Laboratories, Marine Biotechnology Institute
(MBI), Shizuoka, 424, Japan

SOURCE: Experientia (1995), 51(2), 153-5
CODEN: EXPEAM; ISSN: 0014-4754

PUBLISHER: Birkhaeuser

DOCUMENT TYPE: Journal

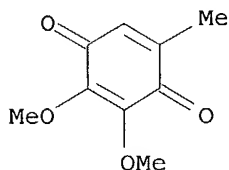
LANGUAGE: English

AB In an attempt to clarify the influence of **marine** bacteria on the settling of fouling invertebrate larvae, we screened for inhibitors, produced by **marine** bacteria, of settling by cyprids of the barnacle, Balanus amphitrite. We found that the culture broth of Alteromonas sp. strain number KK10304, which was associated with the **marine** sponge, Halichondria okadai, effectively inhibited settling of the cyprids. Bioassay-guided isolation indicated ubiquinone-8 as an effective inhibitor of cyprid settling. As ubiquinones are widely distributed in bacteria, several related compds. were also tested.

IT 605-94-7, Ubiquinone-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(ubiquinones from **bacteria** associated with **marine** sponge inhibition of settling of barnacle larvae)

RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



L21 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:666976 HCAPLUS

DOCUMENT NUMBER: 119:266976

TITLE: Organohalogen constituents of the acorn worm
Ptychodera bahamensis

AUTHOR(S): Corgiat, Jay M.; Dobbs, Fred C.; Burger, Mike W.;
Scheuer, Paul J.

CORPORATE SOURCE: Dep. Chem., Univ. Hawaii, Honolulu, HI, 96822, USA

SOURCE: Comparative Biochemistry and Physiology, Part B:
Biochemistry & Molecular Biology (1993), 106B(1), 83-6
CODEN: CBPBB8; ISSN: 0305-0491

DOCUMENT TYPE: Journal

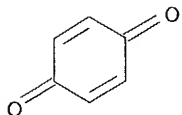
LANGUAGE: English

AB Twenty organohalogen compds., primarily phenols, were detected in the volatile exts. of the acorn worm Ptychodera bahamensis. Five chlorinated compds., previously undescribed from acorn worms, were identified. Enteropneusts can be significant contributors of halogenated orgs. to the **marine** environment.

IT 29533-24-2, Dibromoquinone
RL: BIOL (Biological study)
(in acorn worm)

RN 29533-24-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, dibromo- (9CI) (CA INDEX NAME)



2 (D1-Br)

=> □

=> d his l25

(FILE 'HCAPLUS' ENTERED AT 16:20:04 ON 06 DEC 2004)
L25 36 S (L23 AND L24) NOT (L20 OR L21)

=> d ibib abs hitstr l25 1-36

L25 ANSWER 1 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:710474 HCAPLUS

DOCUMENT NUMBER: 141:391785

TITLE: Quinones as antimycobacterial agents

AUTHOR(S): Tran, Thuyanh; Saheba, Ekta; Arcerio, Ariana V.;
Chavez, Violeta; Li, Qing-yi; Martinez, Luis E.;
Primm, Todd P.

CORPORATE SOURCE: Department of Biological Sciences, The University of
Texas at El Paso, El Paso, TX, 79968, USA

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(18),
4809-4813

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

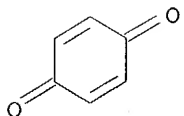
AB Mycobacterium tuberculosis is a serious worldwide health threat, killing almost 3 million people per yr. Other mycobacterial species, especially Mycobacterium avium, are emerging pathogens in the immunocompromised population, most notably AIDS patients. These nontuberculous mycobacteria (NTM) are ubiquitous in the environment, and naturally resistant to many disinfection procedures. Treatment options are limited, and no new antibiotics have been developed against mycobacteria since the 1970s. There is a desperate need for new biocides and antibiotics to prevent and treat mycobacterial infections. A small aromatic compound library has been screened for effectiveness in growth inhibition or killing of mycobacteria. Four species, representing the M. tuberculosis complex, the slow-growing NTM, and the rapid-growing NTM were used. Active compds. had minimal inhibitory concns. as low as 12.5 µg/mL, with the active component being a quinone. The primarily bactericidal activity observed represents a unique mechanism of action. A fluorescent assay involving M. smegmatis expressing gfp was analyzed as a rapid assay for predicting inhibitory activity, but failed to predict activity well. Thus, these compds. may have significant utility as soluble biocides against mycobacteria and other hardy nosocomial pathogens.

IT 106-51-4, 1,4-Benzoquinone, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(quinones as **antimycobacterial** agents)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:362583 HCAPLUS

DOCUMENT NUMBER: 141:106252

TITLE: Synthesis and evaluation of novel 1,4-naphthoquinone derivatives as antiviral, antifungal and anticancer agents

AUTHOR(S): Tandon, Vishnu K.; Singh, Ravindra V.; Yadav, Dharmendra B.

CORPORATE SOURCE: Department of Chemistry, Lucknow University, Lucknow, 226007, India

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2901-2904

CODEN: BMCLE8; ISSN: 0960-894X

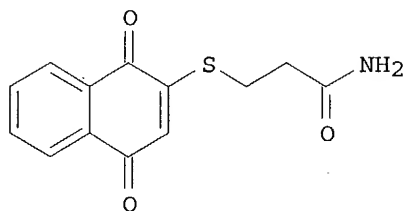
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:106252

GI



I

AB The synthesis and evaluation of some 2-substituted-1,4-naphthoquinones, S-(1,4-naphthoquinon-2-yl)mercaptoalkanoic acid amides, e.g., I, and related quinone derivs., were carried out. The antifungal, antibacterial, antiviral, and anticancer activities were determined by using the standard assay. The results showed that a few of the compds. showed in vitro antiviral activity against Inflenza-A Virus and Herpes Simplex Virus and possess pronounced antifungal profile whereas I showed anticancer activities against Lymphoid Leukemia P 388.

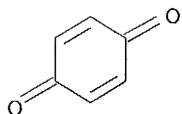
IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation, antifungal, and **antibacterial** activity of carboxypropylsulfanyl- and carboxyphenylsulfanylquinones via condensation of quinones with mercaptopropanoic or mercaptobenzoic acids)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:146768 HCAPLUS

DOCUMENT NUMBER: 140:350028

TITLE: Designing Antibacterial Compounds through a Topological Substructural Approach

AUTHOR(S): Molina, Enrique; Gonzales Diaz, Humberto; Gonzalez, Maykel Perez; Rodriguez, Elismary; Uriarte, Eugenio

CORPORATE SOURCE: Department of Chemistry and Pharmacy Faculty of Engineering Chemistry and Pharmacy, University of Camagueey, Camagueey, 74650, Cuba

SOURCE: Journal of Chemical Information and Computer Sciences (2004), 44(2), 515-521

CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel application of TOPol. Substructural Mol. Design (TOPS-MODE) was carried out in antibacterial drugs using computer-aided mol. design. Two series of compds., one containing antibacterial and the other containing non-antibacterial compds., were processed by a k-means cluster anal. in order to design training and predicting series. All clusters had a p-level < 0.005. Afterward, a linear classification function has been derived toward discrimination between antibacterial and non-antibacterial compds. The model correctly classifies 94% of active and 86% of inactive compds. in the training series. More specifically, the model showed a global good classification of 91%, i.e., 263 cases out of 289. In predicting series, the model has shown overall predictabilities of 91 and 83% for active and inactive compds., resp. Thereby, the model has a global percentage of good classification of 89%. The TOPS-MODE approach, also, similarly compares with respect to one of the most useful models for antimicrobials selection reported to date.

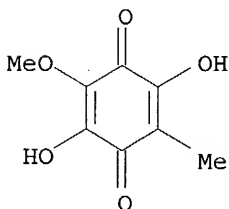
IT 85-23-4 484-89-9, Fumigatin

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(designing antibacterial compds. through a topol. substructural approach)

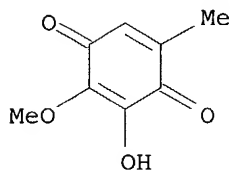
RN 85-23-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3-methoxy-6-methyl- (9CI) (CA INDEX NAME)



RN 484-89-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:2006 HCAPLUS

DOCUMENT NUMBER: 141:54149

TITLE: Chemoselective reaction of bisheterocycle dicarboxylate towards hydrazine hydrate: Synthesis and antimicrobial activity of some new trisheterocycles: 5-pyrrolylaminocarbonyl/oxadiazolyl/mercaptooxadiazolylmethoxy-1-furfuryl-2-methylindoles

AUTHOR(S): Gadaginamath, Guru S.; Donawade, Dundappa S.

CORPORATE SOURCE: Post Graduate Department of Chemistry, Karnatak University, Dharwad, 580 003, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2003), 42B(12), 3108-3112

CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: National Institute of Science Communication

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:54149

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Chemoselectivity of C5-ester over C3-carbethoxy ester function of the bisheterocycle dicarboxylate I (R = OMe) towards the nucleophilic attack of hydrazine hydrate has been evidenced by the exclusive formation of monohydrazide I (R = NH₂NH), which was further reacted with acetonyl acetone, tri-Et orthoformate or carbon disulfide to furnish pyrrolylaminocarbonyl/oxadiazolyl/mercaptooxadiazolylmethoxy furfurylindoles II-IV, resp. The newly synthesized compds. were screened for their antibacterial and antifungal activities.

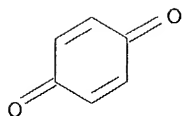
IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of furfurylindoles as **antibacterial** and antifungal agents via chemoselective nucleophilic substitution of furfurylindole dicarboxylate with hydrazine followed by cyclocondensation with hexanedione, orthoester or carbon disulfide)

RN 106-51-4 HCAPLUS

.CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:934746 HCAPLUS

DOCUMENT NUMBER: 138:351053

TITLE: Benzoquinone, the substance essential for antibacterial activity in aqueous extracts from succulent young shoots of the pear *Pyrus* spp.

AUTHOR(S): Jin, Shigeki; Sato, Norio

CORPORATE SOURCE: National Agricultural Research Center for Hokkaido Region, Toyohira-ku, Sapporo, 062-8555, Japan

SOURCE: Phytochemistry (Elsevier) (2003), 62(1), 101-107
CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

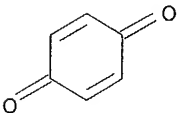
AB Aqueous exts. of the tissue of succulent young shoots of the pear *Pyrus* spp. exhibited strong antibacterial activity against the bacterium *Erwinia amylovora* bv. 4. This activity was investigated quant. by a newly developed bioassay method. It was found that the activity changed with the age of the tissue. Exts. of the youngest leaves and stems from the shoot tops showed the strongest activity, and the activity decreased with age of the leaves and stems. The activity also changed with increase in time after preparation of the extract, increasing rapidly in the first hour after preparation, reaching a maximum at about 4 h, and then decreasing slowly. The substance essential for the antibacterial activity was isolated from the extract by steam distillation in vacuo and through charcoal powder column chromatog. It was identified as benzoquinone (2,5-cyclohexadiene-1,4-dione) by NMR-spectra, mass spectra and HPLC anal. The phenolic metabolism from arbutin to hydroquinone and then to benzoquinone in the aqueous exts. was analyzed quant. by HPLC. The changes in the contents of benzoquinone in the exts. of leaves and stems with tissue aging and with increase in time after preparation of the exts. paralleled the changes in antibacterial activity as determined by the quant. bioassay.

IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); BIOL (Biological study); OCCU (Occurrence) (benzoquinone is essential for **antibacterial** activity in *Pyrus ussuriensis* exts.)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



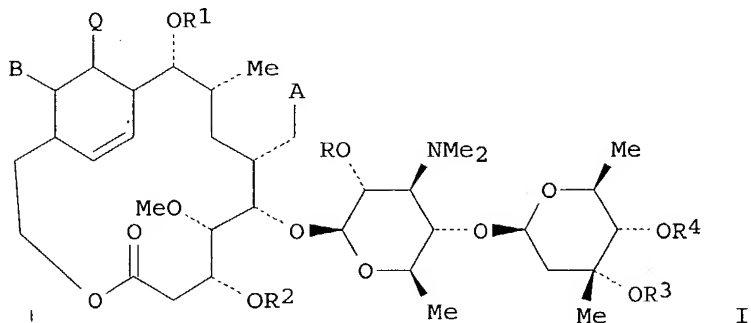
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 6 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:658133 HCAPLUS

DOCUMENT NUMBER: 137:185762
 TITLE: Preparation of aminodeoxy disaccharide bicyclic derivatives of leucomycins as antibacterial agents
 INVENTOR(S): Or, Yat Sun; Binet, Sophie; Phan, Ly Tam
 PATENT ASSIGNEE(S): Enanta Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002066487	A1	20020829	WO 2002-US1427	20020117
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 6462026	B1	20021008	US 2001-785727	20010216
US 2002160966	A1	20021031		
PRIORITY APPLN. INFO.:			US 2001-785727	A 20010216
OTHER SOURCE(S):			MARPAT 137:185762	
GI				

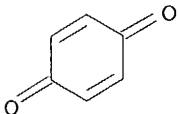


AB Bicyclic leucomycins, e.g. I, were prepared wherein A is CHO, protected aldehyde, CH₂X, X is halogen, amine, amino-carbonyl, sulfonyl, aryloxy, heterocycle-oxy, alkoxy, alkenyloxy, alkynyloxy, heterocycle; B and Q are independently H, ester, acyl, amide, CH₂X, CN, CHO, alkyl, alkenyl, alkynyl; B and Q together are -C(O)YC(O)-; Y is O, substituted C or N; R is H, hydroxy protecting group; R1 and R2 are independently H, OH, protected hydroxy, ester, D-forosamine, L-mycarose; R3 and R4 are independently H, hydroxy protecting group, acyl, and pharmaceutically acceptable compns. comprising a therapeutically effective amount of a compound of the invention in combination with a pharmaceutically acceptable carrier, a method for treating bacterial infectious by administering to a mammal (no data). Thus, I [A = CHO, R = R1 = R3 = H; R2 = Ac, R4 = C(O)CH₂CH(Me)₂, B and Q taken together are C(O)N(Ph)C(O)] was prepared as antibacterial agent (no data).

IT 106-51-4, 1,4-Benzoquinone, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of aminodeoxy disaccharide bicyclic derivs. of leucomycins as
antibacterial agents)

RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 7 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:50135 HCAPLUS

DOCUMENT NUMBER: 137:6102

TITLE: Studies on quinones. Part 35: Access to antiprotozoal
active euryfurylquinones and hydroquinones

AUTHOR(S): Valderrama, Jaime A.; Benites, Julio; Cortes, Manuel;
Pessoa-Mahana, David; Prina, Eric; Fournet, Alain

CORPORATE SOURCE: Facultad de Quimica, Pontificia Universidad Catolica
de Chile, Santiago, Chile

SOURCE: Tetrahedron (2002), 58(5), 881-886

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:6102

AB (+)-Euryfuran adds regiospecifically to activated monosubstituted
1,4-benzoquinones under mild conditions to give the corresponding Michael
adducts which, depending on the quinone substituent, undergo in situ redox
reactions to the resp. euryfurylbenzoquinones. One of these Michael
adducts undergoes a facile stereoselective cyclisation under oxidant
conditions to afford a naphthofuro[4,3-c]benzopyran derivative. The in vitro
activities of the obtained euryfurylquinones and hydroquinones against
Leishmania amazonensis are described. The compds. thus prepared and tested
included (+)-3,6-dihydroxy-2-[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-6,6,9a-
trimethylnaphtho[1,2-c]furan-3-yl]benzaldehyde, (-)-1-[3,6-dihydroxy-2-
[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-6,6,9a-trimethylnaphtho[1,2-c]furan-
3-yl]phenyl]ethanone, 2-acetyl-3-[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-
6,6,9a-trimethylnaphtho[1,2-c]furan-3-yl]-2,5-cyclohexadiene-1,4-dione,
2-[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-6,6,9a-trimethylnaphtho[1,2-
c]furan-3-yl]-3,6-dioxo-1,4-cyclohexadiene-1-carboxylic acid Me ester, and
(-)-(2bS,6aS,7aS)-2b,3,4,5,6,6a,7,7a-octahydro-11-hydroxy-2b,6,6-
trimethylbenzo[b]furo[2,3,4-mn]xanthene-12-carboxaldehyde.

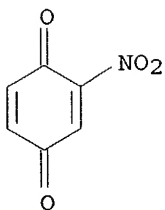
IT 3958-76-7, 2-Nitro-1,4-benzoquinone

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and antiprotozoal activity of (euryfuryl)quinones
(euryfuryl)hydroquinones)

RN 3958-76-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-nitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 8 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:252240 HCAPLUS

DOCUMENT NUMBER: 132:280740

TITLE: Antibacterial paper for safe food packaging

INVENTOR(S): Hara, Kenichi

PATENT ASSIGNEE(S): Daiko Seishi K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF

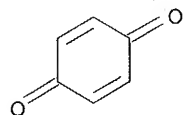
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000110099	A2	20000418	JP 1998-281515	19981002
PRIORITY APPLN. INFO.:			JP 1998-281515	19981002
AB The paper is wet laid from virgin pulp and has been coated with natural extract obtained from bamboo based quinone and tea based catechin.				
IT 106-51-4D, Quinone, compds.				
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)				
(for manufacture of antibacterial paper for safe food packaging)				
RN 106-51-4 HCAPLUS				
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)				



L25 ANSWER 9 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:440809 HCAPLUS

DOCUMENT NUMBER: 131:164556

TITLE: Complexes of 2,5-dihydroxy-1,4-benzoquinone and chloranilic acid with second and third row transition elements

AUTHOR(S): Mostafa, Sahar I.

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Mansoura University, Mansoura, Egypt

SOURCE: Transition Metal Chemistry (Dordrecht, Netherlands) (1999), 24(3), 306-310

CODEN: TMCHDN; ISSN: 0340-4285

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of new 2,5-dihydroxy-1,4-benzoquinone (H2DHBQ) and chloranilic acid (H2CA) complexes cis-[Mo2O5L2]2- (L = DHBQ, CA), [W2O5(DHBQ)2]2-, [WO2(CA)2]2-, trans-[UO2(DHBQ)]·H2O, and trans-[UO2(CA)2]2- is described. Raman, IR, 1H and 13C NMR spectra of the ligands and their complexes are reported and their structures discussed. The antimicrobial activity of the free ligands and several of the complexes was studied.

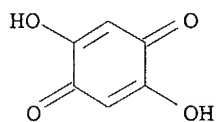
IT 615-94-1, 2,5-Dihydroxy-1,4-benzoquinone

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(antibacterial activity and reactant for preparation of transition metal dihydroxybenzoquinonato complexes)

RN 615-94-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 10 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:265584 HCAPLUS

DOCUMENT NUMBER: 126:248760

TITLE: Bridged diphenyl compounds as drugs against parasitic protozoa

INVENTOR(S): Winter, Rolf Walter; Riscoe, Michael Kevin; Hinrichs, David J.

PATENT ASSIGNEE(S): Interlab Corporation, USA

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

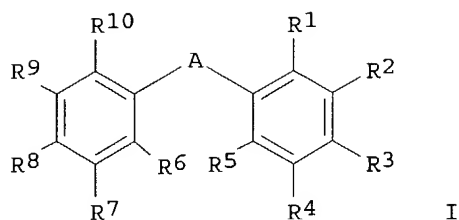
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9707790	A1	19970306	WO 1996-US13672	19960823
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
AU 9668589	A1	19970319	AU 1996-68589	19960823
PRIORITY APPLN. INFO.:			US 1995-520694	A 19950828
			WO 1996-US13672	W 19960823

OTHER SOURCE(S): MARPAT 126:248760

GI

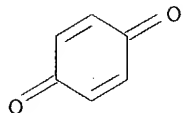


AB The synergistic combination of certain bridged di-Ph compds. [I; A = C(O), O, NH, S, S(O), SO₂, C:C, NR, CX₁X₂; R, X₁, X₂ = H, OH, (halo)alkyl, (halo)alkylamino; R₁-R₁₀ = H, OH, halo, OAc, OMe, NH₂, SO₃⁻, N₃, (halo)alkyl, alkylamino, aminoalkoxy, CO₂X₃; X₃ = H, alkyl] with oxidants for the treatment of infectious diseases caused by protozoa is disclosed. Thus, the inhibition of growth of Plasmodium falciparum in vitro by rufigallol was potentiated 350-fold by 2,3,4,3',4',5'-hexahydroxybenzophenone (exifone).

IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (bridged di-Ph compds. as drugs against parasitic protozoa)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 11 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:646431 HCAPLUS

DOCUMENT NUMBER: 123:165058

TITLE: Fungitoxic compounds from the roots of tomato stock

AUTHOR(S): Nagaoka, Toshinori; Ohra, Junko; Yoshihara, Teruhiko; Sakamura, Sadao

CORPORATE SOURCE: Fac. Appl. Biol. Sci., Hiroshima Univ., Higashihiroshima, 724, Japan

SOURCE: Nippon Shokubutsu Byori Gakkaiho (1995), 61(2), 103-8
 CODEN: NSBGAM; ISSN: 0031-9473

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fungitoxic compds. from the roots of tomato stocks, Taibyo Shinko Number 1, were determined as 4 unsatd. hydroxy fatty acids, (13S)-13-hydroxy-(9Z,11E)-9,11-octadecadienoic acid, 13-hydroxy-(9E,11E)-9,11-octadecadienoic acid, (9S)-9-hydroxy-(10E,12Z)-10,12-octadecadienoic acid and 9-hydroxy-(10E,12E)-10,12-octadecadienoic acid, a dicarboxylic acid (azelaic acid), a quinone (2,6-dimethoxy-p-benzoquinone) and 5 phenolic compds. (vanillin, syringaldehyde, p-hydroxybenzaldehyde, p-hydroxybenzoic acid, vanillic acid). It can be considered that the fungitoxic compds. related to resistance of the tomato stock against soil-borne disease were alkaloids, but not these universal compds. in plants.

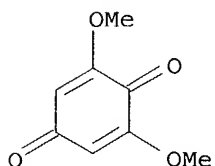
IT 530-55-2

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(fungitoxic compds. from roots of tomato stock)

RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)



L25 ANSWER 12 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:604351 HCAPLUS

DOCUMENT NUMBER: 123:8036

TITLE: Manufacture of antibacterial and antifungal substances from syringaldehyde with peroxidase and antibacterial and antifungal agents containing the substances

INVENTOR(S): Kobayashi, Akio; Oguchi, Yasushi; Kanzaki, Hiroshi; Kajama, Shinichiro; Kawazu, Kazuyoshi

PATENT ASSIGNEE(S): Kibun Shokuhin Kk, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

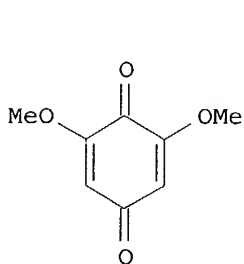
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

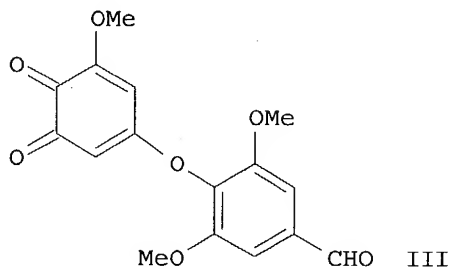
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

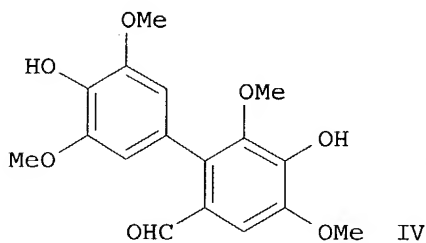
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07076547	A2	19950320	JP 1993-223415	19930908
JP 3529814	B2	20040524		
PRIORITY APPLN. INFO.: GI			JP 1993-223415	19930908



II



III



IV

AB Antibacterial and antifungal substances are manufactured by treatment of syringaldehyde (I) with peroxidase in the presence of H2O2. I was

incubated with peroxidase and H₂O₂ at 25° and pH 5.8 for .apprx.3 h to manufacture a quinone II, a Ph ether III, and a biphenyl compound IV. II, III, and IV inhibited Escherichia coli with min. inhibitory concns. of 63, 500, and 500 µg/mL, resp.

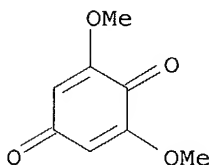
IT 530-55-2P

RL: BAC (Biological activity or effector, except adverse); BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)

(manufacture of **antibacterial** and antifungal compds. with peroxidase and H₂O₂ from syringaldehyde)

RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)



L25 ANSWER 13 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:451619 HCAPLUS

DOCUMENT NUMBER: 121:51619

TITLE: Expert-system comparison of structural determinants of chemical toxicity to environmental bacteria

AUTHOR(S): Pangrekar, Jyotsna; Klopman, Gilles; Rosenkranz, Herbert S.

CORPORATE SOURCE: Grad. Sch. of Public Health, Univ. Pittsburgh, Pittsburgh, PA, 15261, USA

SOURCE: Environmental Toxicology and Chemistry (1994), 13(6), 979-1001

CODEN: ETOCDK; ISSN: 0730-7268

DOCUMENT TYPE: Journal

LANGUAGE: English

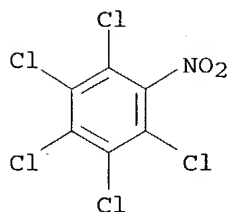
AB The CASE (computer automated structure evaluation) structure-activity relational expert system was used to analyze the toxicity of a database of chemical sets to environmental bacteria (aerobic heterotrophs, nitrosomonas, methanogens, and photobacteria [Microtox test]). The anal. revealed that the data sets related to each of the antimicrobial activities, albeit containing a relatively small number of chems., are characterized by structural determinants significantly associated with the probability of antimicrobial activity, as well as with antibacterial potency. Although there were a number of similarities among the structural determinants associated with each of these antimicrobial activities, there were also features unique to each assay that presumably reflect species-specific targets of bactericidal activity. Overall the assay for antimethanogenic activity appears to be the most informative as well as the one most predictive of the activity in the other three assays.

IT 82-68-8, Pentachloronitrobenzene 106-51-4, 1,4-Benzoquinone, biological studies

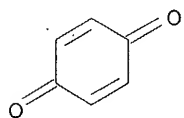
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to environmental **bacteria**, expert system in study of)

RN 82-68-8 HCAPLUS

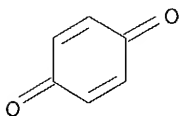
CN Benzene, pentachloronitro- (8CI, 9CI) (CA INDEX NAME)



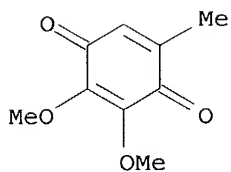
RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



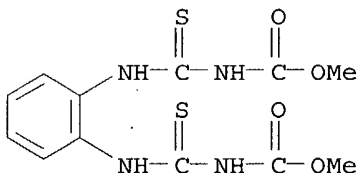
L25 ANSWER 14 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:210628 HCAPLUS
DOCUMENT NUMBER: 120:210628
TITLE: Detection of herbicides via a bacterial photoreaction center and bacterial luciferase
AUTHOR(S): Jockers, Ralf; Schmid, Rolf D.
CORPORATE SOURCE: Proj. Group Biosens., GBF--Ges. Biotechnol. Forsch. mbH, Braunschweig, D(W)-3300, Germany
SOURCE: Biosensors & Bioelectronics (1993), 8(6), 281-9
CODEN: BBIOE4; ISSN: 0956-5663
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new detection principle for ligands (photosystem-II herbicides) based on bacterial luciferase as the detection system is presented. The dependency of luciferase on long-chain aliphatic aldehydes was used. The requirements for such a system are investigated. Studies were made of the binding properties of artificial aldehydes to the QB-binding site of photoreaction centers from the phototrophic bacteria Rhodobacter sphaeroides and substrate properties for bacterial luciferase from Photobacterium fischeri of various artificial aldehydes.
IT 106-51-4, 1,4-Benzoquinone, biological studies 605-94-7, Ubiquinone 0
RL: PROC (Process)
(binding of, to QB site of bacterial photoreaction center)
RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



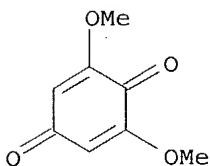
RN 605-94-7 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



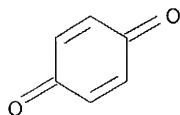
L25 ANSWER 15 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1994:25511 HCAPLUS
 DOCUMENT NUMBER: 120:25511
 TITLE: Naturally occurring antidotes against benzimidazole fungicides
 AUTHOR(S): Tahara, Satoshi; Matsukura, Yumiko; Katsuta, Hiroyuki; Mizutani, Junya
 CORPORATE SOURCE: Fac. Agric., Hokkaido Univ., Sapporo, 060, Japan
 SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1993), 48(9-10), 757-65
 CODEN: ZNCBDA; ISSN: 0341-0382
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB TLC bioautog. using precoated glass thin-layer plates impregnated with benomyl or carbendazim (MBC), and Cladosporium herbarum as a test fungus, was evaluated as a facile way to detect plant secondary metabolites antidoting against benzimidazole fungicides. In addition to emodin and α -tocopherol from Polygonum sachalinense, three phenolics, 3,5-dihydroxy-4-methylstilbene and 5-methoxy-6,7-methylenedioxyflavone from P. lapathifolium and 2,6-dimethoxybenzoquinone from P. thunbergii, were isolated and characterized as new benzimidazole antidotes. Emodin exhibited the antidoting activity not only against benomyl but also against MBC, thiabendazole, thiophanate-Me and nocodazole. Furthermore, emodin showed antidoting activity against MBC in the wild-type Neurospora crassa and against diethofencarb in the mutant of N. crassa resistant to benzimidazole fungicides but highly susceptible to diethofencarb.
 IT 23564-05-8, Thiophanate-methyl
 RL: BIOL (Biological study)
 (antidotes against, emodin as)
 RN 23564-05-8 HCAPLUS
 CN Carbamic acid, [1,2-phenylenebis(iminocarbonothioyl)]bis-, dimethyl ester (9CI) (CA INDEX NAME)



IT 530-55-2
 RL: BIOL (Biological study)
 (benzimidazole fungicide antidote, from Polygonum thunbergii)
 RN 530-55-2 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)



L25 ANSWER 16 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1993:555979 HCAPLUS
 DOCUMENT NUMBER: 119:155979
 TITLE: Inhibition of *Mucor rouxii* growth by synthetic substances
 AUTHOR(S): Sabanero, Myrna; Rojas, Emma; Torres, Veronica; Farfan, Norberto; Contreras, Rosalinda
 CORPORATE SOURCE: Fac. Quim., Univ. Guanajuato, Mex.
 SOURCE: Revista Latinoamericana de Microbiologia (1991), 33(4), 297-303
 CODEN: RLMIAA; ISSN: 0034-9771
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Micor rouxii cells were used to examine the possible antimycotic activities of 4 substances: phenolamines, phenylenediamine and quinone. These substances are original structures recently synthesized. Assays in plates showed that 10-2 M of phenolamines and phenylenediamines give rise to halos of growth inhibition. Assays in liquid media using 10-4 M of substances showed 100% inhibition of spore germination. Specifically, the phenylenediamine showed 49% inhibition on development of mycelium. In these cells the calcofluor distribution changes, suggesting alterations in cell wall. No inhibition of growth was found using the quinone. The activity for substances were evaluated using standard antifungal benomyl. On this basis, phenylendiamine is antimycotically active. The mechanism of action is not presently known.
 IT 106-51-4P, Quinone, preparation
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and **fungicidal** activity of)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



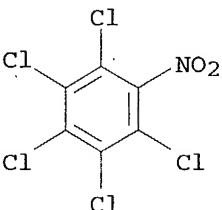
L25 ANSWER 17 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1991:508064 HCAPLUS
 DOCUMENT NUMBER: 115:108064
 TITLE: A database of chemical toxicity to environmental bacteria and its use in interspecies comparisons and correlations
 AUTHOR(S): Blum, Diane J. W.; Speece, R. E.
 CORPORATE SOURCE: Bala Cynwyd, PA, 19004, USA
 SOURCE: Research Journal of the Water Pollution Control Federation (1991), 63(3), 198-207
 CODEN: RJWFE7; ISSN: 1047-7624

DOCUMENT TYPE: Journal
 LANGUAGE: English

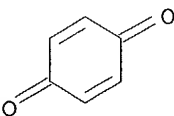
AB This research assayed the toxicity of 50-100 chems. to each of 3 bacterial groups: aerobic heterotrophs, Nitrosomonas, and methanogens. Chems. tested comprise important environmental pollutants such as chlorinated aliphatic hydrocarbons and halogenated and other substituted benzenes and phenols. Toxicity data were obtained from the literature for fathead minnows and for the Microtox test for comparison with author's bacterial data. Aerobic heterotrophs and methanogens showed similar sensitivities to toxicants, with the exception of an enhanced susceptibility of methanogens to chlorinated aliphatic hydrocarbons and alcs. Nitrosomonas, Microtox, and the fathead minnow showed similar sensitivities as one another, which were one order of magnitude greater than the sensitivities of the aerobic heterotrophs and methanogens. Correlations among the toxicities to different organisms allow predictions of a chemical toxicity to one organism to be made based on the toxicity of that chemical to a different organism. Excellent correlations were found between chemical toxicities to the aerobic heterotrophs, methanogens (with chlorinated aliphatic hydrocarbons omitted), and fathead minnows. Good correlations were found between Microtox and each of the other bacteria and the fathead minnow.

IT 82-68-8 106-51-4, 1,4-Benzoquinone, biological studies
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (toxicity of, to environmental **bacteria**, species in relation to)

RN 82-68-8 HCAPLUS
 CN Benzene, pentachloronitro- (8CI, 9CI) (CA INDEX NAME)



RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 18 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1991:22693 HCAPLUS
 DOCUMENT NUMBER: 114:22693
 TITLE: Microbicidal agents containing benzoquinones for foods
 INVENTOR(S): Nishina, Atsuro; Ito, Masaji
 PATENT ASSIGNEE(S): Nippon Oil and Fats Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokyo Koho, 2 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

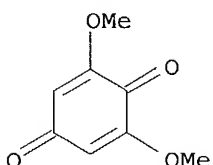
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02202804	A2	19900810	JP 1989-20796	19890201
PRIORITY APPLN. INFO.:			JP 1989-20796	19890201

AB Microbicidal agents contain benzoquinones as effective components. The benzoquinones are safe and inexpensive, have a broad spectrum of activity, and are useful for foods. Min. inhibitory concentration values of methyl-p-benzoquinone, 2,3-dimethoxy-5-methyl-p-benzoquinone, and 2,6-dimethoxy-p-benzoquinone against various bacteria and fungi are given.

IT 530-55-2, 2,6-Dimethoxy-p-benzoquinone 553-97-9, Methyl-p-benzoquinone 605-94-7, 2,3-Dimethoxy-5-methyl-p-benzoquinone
 RL: BIOL (Biological study)
 (bactericide and fungicide, for foods)

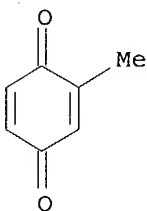
RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)



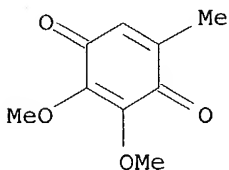
RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



L25 ANSWER 19 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:402345 HCAPLUS

DOCUMENT NUMBER: 109:2345

TITLE: In vitro evaluation of some natural products for their fungitoxicity

AUTHOR(S): Dube, S.; Shukla, H. S.; Tripathi, S. C.

CORPORATE SOURCE: Dep. Bot., Univ. Gorakhpur, Gorakhpur, 273009, India

SOURCE: Pesticides (1988), 22(3), 11-12

CODEN: PSTDAN; ISSN: 0031-6148

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Of 18 natural products, benzoquinone, m-chloroaniline, and o-cresol were the most effective against *Aspergillus flavus*. At 500 ppm they inhibited mycelial growth by 90%. At 700 ppm, these compds., as well as camphor, catechol, and p- and m-cresol, totally suppressed the growth. Me imparted higher effectiveness to the phenol ring than did either NH₂ or COOH. Amino group at the phenol ring was more effective at ortho than at the para or meta positions. Two or more OH groups also increased the antifungal potency.

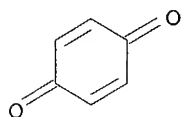
IT 106-51-4, biological studies

RL: BIOL (Biological study)

(fungitoxicity of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 20 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1986:507995 HCAPLUS

DOCUMENT NUMBER:

105:107995

TITLE:

Respiratory inhibition by the antifungal benzoquinone, 2-hydroxy-6-methoxy-3,5-dimethyl-1,4-benzoquinone
Haraguchi, Hiroyuki; Soga, Osamu; Taniguchi, Makoto
Fac. Sci., Osaka City Univ., Osaka, 558, Japan
Agricultural and Biological Chemistry (1986), 50(7), 1905-7

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

CODEN: ABCHA6; ISSN: 0002-1369

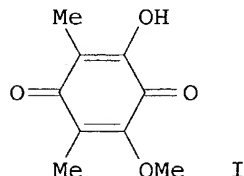
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI



AB The title antifungal compound I [76186-46-4] lowered the respiratory-control but not the ADP/O ratio of rat liver mitochondria (used instead of the more unstable fungal mitochondria) incubated with α -ketoglutarate and succinate as the respiratory substrates. I depressed the state-3 but not state-4 respiration rate in 2,4-dinitrophenol-uncoupled mitochondria. Also, I inhibited succinate-[9028-10-8] and NADH-cytochrome C reductase [9027-14-9]. Thus, the site of respiration inhibition by I appears to be in the electron-transport system. The effect of I on mitochondria may be related to its antifungal action. The antimicrobial potency of I against several **bacteria**

and **fungi** in vitro was also studied.

L25 ANSWER 21 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:58267 HCAPLUS

DOCUMENT NUMBER: 102:58267

TITLE: Mediator function of biologically active n-type quinones in a peroxidase enzymic reaction initiated electrochemically

AUTHOR(S): Shapovalov, V. A.

CORPORATE SOURCE: Khar'k. Gos. Farm. Inst., Kharkov, USSR

SOURCE: Elektrokimiya (1984), 20(10), 1383-5

CODEN: ELKKAX; ISSN: 0424-8570

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The electrochem. reduction of quinone derivs. during the reaction of peroxidase with H₂O₂ was investigated, and the physiol. effectiveness of the derivs. as fungicides was compared to their ability to stimulate the peroxidase reaction. The time for conversion of 1/2 of the available H₂O₂ by the enzyme in the presence of the quinone derivs. ($\tau_{1/2}$) correlated well with their fungicidal activities. Furthermore, the limiting current for electrochem. reduction of the quinones in the presence of enzyme also correlated with the $\tau_{1/2}$. Thus, the electrochem. reduction of quinones in the presence of peroxidase may constitute a screening procedure for the fungicidal activity of quinones.

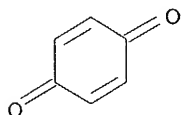
IT 106-51-4, reactions 106-51-4D, derivs.

RL: RCT (Reactant); RACT (Reactant or reagent)

(electrochem. reduction of, in peroxidase presence, **fungicidal** activity in relation to)

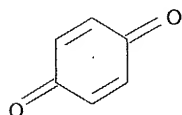
RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 22 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:503756 HCAPLUS

DOCUMENT NUMBER: 91:103756

TITLE: Methylbenzoquinone fungicides

INVENTOR(S): Watanabe, Yoshihachi; Iwao, Toru

PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 2 pp.

CODEN: JKXXAF

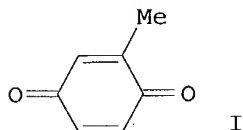
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54067027	A2	19790530	JP 1977-132920	19771104
PRIORITY APPLN. INFO.: GI			JP 1977-132920	19771104

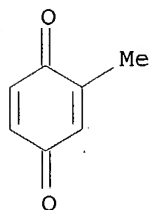


AB 2-Methyl-1,4-benzoquinone (I) [553-97-9] controls soil phytopathogens. Thus, 1000 ppm I controlled *Phythium aphanidematum*, *Rhizoctonia solani*, and *Fusarium oxysporum* in soil.

IT 553-97-9
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
 (fungicides)

RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



L25 ANSWER 23 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:501628 HCAPLUS

DOCUMENT NUMBER: 89:101628

TITLE: In vitro effect of some phenols, quinones and growth hormones on the fungal pathogens causing wilt of gram (*Cicer arietinum* L.)

AUTHOR(S): Mathur, Sunila; Chauhan, S. K.

CORPORATE SOURCE: Sch. Stud. Bot., Vikram Univ., Ujjain, India

SOURCE: Proceedings of the National Academy of Sciences, India, Section B: Biological Sciences (1976), 46(4), 491-4

CODEN: PAIBA6; ISSN: 0369-8211

DOCUMENT TYPE: Journal

LANGUAGE: English

AB PhOH [108-95-2], catechol [120-80-9], pyrogallol [87-66-1], benzoquinone [106-51-4], IAA [87-51-4], 2,4-D [94-75-7], 2-naphthoxyacetic acid [120-23-0], NAA [86-87-3], biotin [58-85-5], thiamin [59-43-8], and inositol [87-89-8] were tested for their fungicidal properties against *Fusarium oxysporum*, *Rhizotonia solani* and *Sclerotium rolfsii*, causing wilt of gram (*C. arietinum*), at 10, 50, and 100 ppm. These compds. caused different effects on the growth of the pathogens as revealed by the difference in colony diams., dry mycelial

weight and percentage germination of spores (only in the case of *Fusarium*). Benzoquinone, PhOH, catechol, pyrogallol, thiamin, and IAA were effective against *F. oxysporum* and catechol and IAA against *R. solani* and *S. rolfsii*.

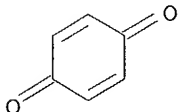
IT 106-51-4, biological studies

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicide, for gram wilt control)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 24 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:578837 HCAPLUS

DOCUMENT NUMBER: 87:178837

TITLE: The effect on fungal growth of some 2,5-dihydroxy-1,4-benzoquinones

AUTHOR(S): Brewer, D.; Maass, W. S. G.; Taylor, A.

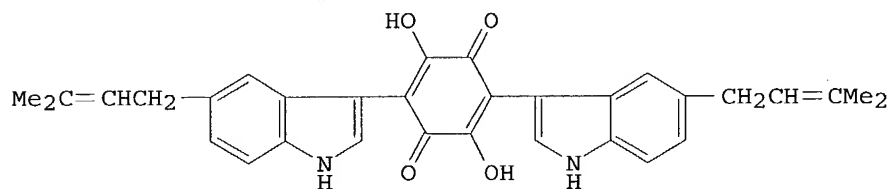
CORPORATE SOURCE: Natl. Res. Counc. Canada, Halifax, NS, Can.

SOURCE: Canadian Journal of Microbiology (1977), 23(7), 845-51
CODEN: CJMIAZ; ISSN: 0008-4166

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB 2,5-Dihydroxy-1,4-benzoquinones decreased vegetative growth and inhibited spore germination of 12 species of fungi belonging to 6 diverse genera. The nature of the substituents at the 3 and 6 positions of the quinone ring affected their growth-inhibitory properties; generally those substituents of lower polarity inhibited growth at lower concns. As in the case of cochliodinol (I) [11051-88-0], chemical modification of the quinone group, or the hydroxyl groups of the quinone ring, in compds. of the polyporic acid series, also led to loss of biol. activity.

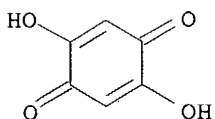
IT 615-94-1D, derivs.

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicidal activity of)

RN 615-94-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy- (9CI) (CA INDEX NAME)



L25 ANSWER 25 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:414559 HCAPLUS

DOCUMENT NUMBER: 85:14559

TITLE: Studies on fungal products. Part IV. Isolation of oospolactone as the antifungal principle of *Gloeophyllum sepiarium*

AUTHOR(S): Nakajima, Shoichi; Kawai, Kenichi; Yamada, Shizue; Sawai, Yuko

CORPORATE SOURCE: Hoshi Coll. Pharm., Tokyo, Japan

SOURCE: Agricultural and Biological Chemistry (1976), 40(4), 811-12

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Oospolactone (3,4-dimethyl-8-hydroxyisocoumarin) [1570-27-0], isolated from *G. sepiarium* cultures, was active against a wide variety of fungi. Along with oospolactone, 2,5-dimethoxy-p-benzoquinone [3117-03-1], methyl sulphrenate [19683-37-5], and ergosteryl palmitate [3992-98-1] were isolated.

L25 ANSWER 26 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:116867 HCAPLUS

DOCUMENT NUMBER: 84:116867

TITLE: Fungitoxicity and insecticide synergism of monothioquinol phosphate esters and related compounds

AUTHOR(S): Eto, Morifusa; Hashimoto, Yasuaki; Ozaki, Kozaburo; Kassai, Tatsuo; Sasaki, Yoshitaka

CORPORATE SOURCE: Dep. Agric. Chem., Kyushu Univ., Fukuoka, Japan

SOURCE: Bochu Kagaku (1975), 40(3), 110-17

CODEN: BOCKAF; ISSN: 0006-5420

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Of O-Et S,S-di-Ph phosphorodithioate [17109-49-8], 4 phosphorothioates (EtO)2P(O)SC6H4R-4 (R = OH, OMe, OCO2Et, or Me), and 9 phosphates (R1O)2P(O)OR2 (R1 = Et or Ph, R2 = substituted Ph) synthesized, only the phosphorothioates and the phosphorodithioate showed fungitoxic activity against *Aspergillus niger*, in vitro. Some hydrolysis products, such as Ph disulfide [882-33-7] and p-hydroxythiophenol [637-89-8] were more fungitoxic than the parent esters. There was a correlation between the fungitoxic activity, and the lipophilic character, as expressed by the partition coefficient, for some of the compds. None of the compds. inhibited at 5 + 10-4M, the respiration of *A. niger*, whereas some oxidized derivs. of the hydrolysis products, such as inhibitory had a strong inhibitory activity. Tri-Ph phosphate [115-86-6] and di-Et S-ethoxycarbonyloxyphenyl phosphorothioate [40249-48-7] synergized the insecticidal activity of malathion [121-75-5] against malathion-resistant strain of *Laodelphax striatellus*. The phosphorothioates synergized malathion much more than did tri-Ph phosphate against the green rice leafhopper (*Nephotettix cincticeps*). Tri-Ph phosphate, di-Et 4-hydroxyphenyl phosphate [13953-88-3] and O,O-di-Et S-ethoxycarbonyloxyphenyl phosphorothioate synergized the insecticidal activity of carbaryl [63-25-2] against the tobacco cutworm (*Prodenia litura*), but less than did piperonyl butoxide.

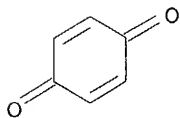
IT 106-51-4, biological studies

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicidal activity of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



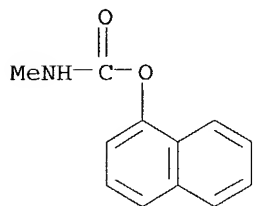
IT 63-25-2 121-75-5

RL: BIOL (Biological study)

(insecticidal synergism with, by phosphates and phosphorothiolates)

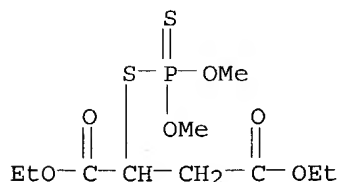
RN 63-25-2 HCAPLUS

CN 1-Naphthalenol, methylcarbamate (9CI) (CA INDEX NAME)



RN 121-75-5 HCAPLUS

CN Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester (9CI)
(CA INDEX NAME)



L25 ANSWER 27 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:93975 HCAPLUS

DOCUMENT NUMBER: 60:93975

ORIGINAL REFERENCE NO.: 60:16440c

TITLE: Quinone as a fungicide. The history of its investigation and a view of its mode of action

AUTHOR(S): Braune, Wolfram

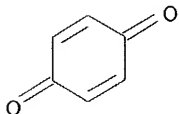
CORPORATE SOURCE: Friedrich-Schiller Univ., Jena, Germany

SOURCE: Zentralblatt fuer Bakteriologie, Parasitenkunde, Infektionskrankheiten und Hygiene, Abteilung 2, Naturwissenschaftliche: Allgemeine, Landwirtschaftliche und Technische Mikrobiologie (1964), 117(4), 412-24
CODEN: ZBPIA9; ISSN: 0044-4057

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB A review with many references.
 IT 106-51-4, p-Benzoquinone
 (fungicidal action of)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

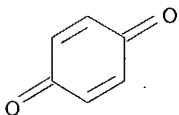


L25 ANSWER 28 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1960:104762 HCAPLUS
 DOCUMENT NUMBER: 54:104762
 ORIGINAL REFERENCE NO.: 54:19969a-c
 TITLE: The effects of benzothiazole derivatives and some
 others upon Candida in vitro
 AUTHOR(S): Toda, Tadao; Tokunaga, Toru
 CORPORATE SOURCE: Univ. Kyushu
 SOURCE: Chemotherapy (Tokyo) (1959), 7, 332-5
 CODEN: NKRZAZ; ISSN: 0009-3165
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB The growth-inhibitory activity toward Candida albicans, C. krusei, C. guilliermondi and several bacterial strains was examined in vitro of 6-carboxy-, 6-ethoxycarbonyl-, 6-carboxymethoxy-, 6-cyano-, 4,7-dichloro-6-cyano-, 4,7-dichloro-6-carboxy-, 6-carbamoyl-, and the HCl salt of 6-hydrazino carbonyl-2-methylbenzothiazole, 2-methylbenzothiazole-6-carbonylhydrazones of benzoquinone, 3-chlorobenzoquinone, quinoxime and 2-isopropyl-5-methylquinoxime, 6-methyl- and 6-ethoxycarbonyl-2-aminobenzothiazole, 2-acetamido-6-methyl-benzothiazole, monochlorobenzoquinone, 2,5-dichloro-4-thiocyanatoaniline (I), bis(2,5-dichloro-4-aminophenyl) disulfide, Et 3-thiocyanato-4-aminobenzoate, and nitrosothymol. All of benzothiazole derivs. were not so effective, but I had a high growth-inhibitory power against not only Candida, but also bacteria generally. I was highly bacteriostatic against Mycobacterium tuberculosis including streptomycin and isonicotinoyl hydrazide (II)-resistant strains. Its acute toxicity in mice was much lower than II.

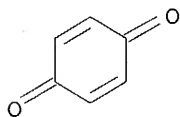
IT 106-51-4, p-Benzoquinone
 (hydrazones with 2-methyl-6-benzothiazolecarboxylic acid hydrazide,
 bactericidal and fungicidal action of)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 29 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1958:16486 HCAPLUS
 DOCUMENT NUMBER: 52:16486
 ORIGINAL REFERENCE NO.: 52:3014d-f
 TITLE: Effects of some phenols and quinones on growth in
 vitro of Verticillium albo-atrum

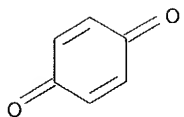
AUTHOR(S): LeTourneau, Duane; McLean, John G.; Guthrie, James W.
 CORPORATE SOURCE: Idaho Agr. Expt. Sta., Moscow
 SOURCE: Phytopathology (1957), 47, 502-6
 CODEN: PHYTAJ; ISSN: 0031-949X
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB The effects of 13 phenols and phenolic acids and 4 quinones on the growth in liquid medium of *V. albo-atrum* were determined. Of 3 isomeric dihydroxybenzenes, catechol (I) was most inhibitory. Replacement of an OH group with a COOH group or the introduction of a COOH group on the ring decreased the effectiveness of I. Pyrogallol was the most toxic phenolic compound tested. The quinones were generally more inhibitory than the phenols. 1,4-Naphthoquinone was more inhibitory than 1,4-benzoquinone, and chlorination of the quinones increased their inhibitory action. 2,3-Dichloro-1,4-naphthoquinone caused appreciable growth inhibition at a concentration of 10⁻⁶M.
 IT 106-51-4, p-Benzoquinone
 (as **fungicide** for *Verticillium albo-atrum*)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 30 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1955:62269 HCAPLUS
 DOCUMENT NUMBER: 49:62269
 ORIGINAL REFERENCE NO.: 49:11947a-c
 TITLE: Fungicidal preparations
 INVENTOR(S): Tjepkema, Jacobus J.; Montagne, Johannes Th. W.
 PATENT ASSIGNEE(S): .N. V. de Bataafsche Petroleum Maatschappij
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 76833		19541215	NL	
AB	New and valuable fungicides have been found in 1,4-benzoquinones and 1,4-naphthoquinones where the first type carries 2 or 4 alkylthio groups, the latter 2 alkylthio groups. They are used in the form of aqueous emulsions of solns. of the compds. in hydrocarbon oils. Because of their good solubility in mineral oil they can be applied by the method of low-volume spraying. E.g. for 2,3-bis(isopropylthio)-1,4-naphthoquinone the solubility is 3% and the L.D.50 is 2.5 p.p.m.; for 2,3,5,6-tetrakis(isoamylthio)-1,4-benzoquinone the solubility is 25% and the L.D.50 is 20 p.p.m., as measured by the "Slide germination method".			
IT	106-51-4, p-Benzoquinone (derivs., for fungicides)			
RN	106-51-4 HCAPLUS			
CN	2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)			



L25 ANSWER 31 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1955:30526 HCAPLUS

DOCUMENT NUMBER: 49:30526

ORIGINAL REFERENCE NO.: 49:5848h

TITLE: Preparation of microbiologically resistant wool by chemical modification. VI. Benzoquinone, ninhydrin, and heavy metal salts

AUTHOR(S): Zahn, Helmut; Wurz, Albrecht; Rauchle, Adolf

CORPORATE SOURCE: Univ. Heidelberg, Germany

SOURCE: Textile Research J. (1955), 25, 120-4

DOCUMENT TYPE: Journal

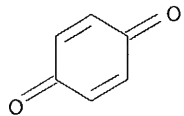
LANGUAGE: Unavailable

AB The beneficial effects of these compds. are noted. Treatment with bis(chloromethyl)benzene protects against attack by bacteria, moths, and alkali. Possibilities for com. applications are suggested.

IT 106-51-4, p-Benzoquinone
(wool proofing against **bacteria** and **fungi** by)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 32 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1954:40456 HCAPLUS

DOCUMENT NUMBER: 48:40456

ORIGINAL REFERENCE NO.: 48:7243f-h

TITLE: Fungicidal action. II. Constitution of benzenoid and quinonoid compounds in relation to fungitoxicity and inhibition of amino- and sulfhydryl-dependent enzymes

AUTHOR(S): Owens, Robert G.

SOURCE: Contributions from Boyce Thompson Institute (1953), 17, 273-82

CODEN: CBTIAE; ISSN: 0006-8543

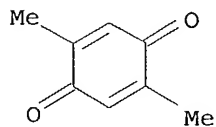
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

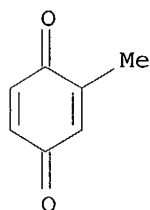
AB cf. McNew and Burchfield, C.A. 46, 11543a. The inhibition of pancreatic and malt amylases was compared with the ED50 value against Alternaria oleracea and Monilinia fructicola. Inhibitory effects and fungicidal effects were correlated with durene, 4-nitroveratrole, veratrole, hydroquinone dimethyl ether, hydroquinone diethyl ether, guaiacol, resorcinol, catechol, di-tert-amylhydroquinone, toluhydroquinone, 2,5-dichlorohydroquinone, p-benzoquinone, tolu-p-benzoquinone, chloranilic acid, 2,5-dichloroquinone, 2,6-dichloroquinone, and 2,6-dichloroquinone chloroimide. 2,4-Dichlorotoluene, 3,4-dichlorotoluene, hydroquinone monomethyl ether, p-xyloquinone, 1,4-naphthoquinone, 2-methyl-1,4-naphthoquinone, and 2,3-dichloro-1,4-naphthoquinone were more active against the fungi than against the enzymes. Hydroquinone, tetrachloro-p-benzoquinone, and 1,2-naphthoquinone were more active

against the enzymes.

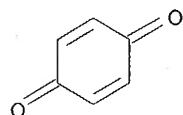
IT 137-18-8, Phlorone 553-97-9, p-Toluquinone
(fungitoxicity of and enzyme inhibition by)
RN 137-18-8 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dimethyl- (9CI) (CA INDEX NAME)



RN 553-97-9 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



IT 106-51-4, p-Benzoquinone
(fungitoxicity of, and enzyme inhibition by)
RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 33 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

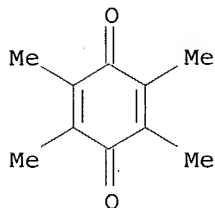
ACCESSION NUMBER: 1953:7439 HCAPLUS
DOCUMENT NUMBER: 47:7439
ORIGINAL REFERENCE NO.: 47:1326c-e
TITLE: Fungicidal and insecticidal preparations containing
halogenated duroquinone
INVENTOR(S): Schmidl, Albert U.
PATENT ASSIGNEE(S): Standard Oil Development Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2615827		19521028	US	

AB Halogenation of duroquinone (I) in the presence of light and(or) a halogen carrier is controlled until I contains an average of more than 50% by weight of halogen on the nonaromatic C atoms. When the slide germination method is used, a solution of 0.001-0.0001 weight % of chlorinated duroquinone (II) containing 54.5% by weight of Cl allowed only 50% germination to Alternaria solani and

Sclerotinia fructiola. Immersion of a milk-weed bug for 2 min. in a 0.25 weight % suspension of II produces 100% mortality. The same treatment produces 30% mortality of the German roach. Injection of 0.5 mg. of II per g. of body weight into the blood stream of the American roach results in 100% mortality. When the Nelson drop test is used, a suspension of II results in 95% mortality of the housefly. Halogenated I exhibits no phytotoxicity on coleus.

IT 527-17-3, p-Benzoquinone, tetramethyl-
(chlorinated, fungicides and insecticides from)
RN 527-17-3 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)

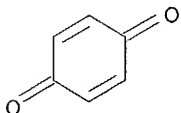


L25 ANSWER 34 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

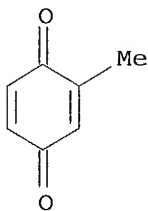
ACCESSION NUMBER: 1952:52712 HCAPLUS
DOCUMENT NUMBER: 46:52712
ORIGINAL REFERENCE NO.: 46:8779c-g
TITLE: Antiseptics for foods. LI
AUTHOR(S): Fujikawa, Fukujiro; Tokuoka, Akimasa; Takimura, Miyoko; Miura, Kazuko
CORPORATE SOURCE: Kyoto Coll. Pharm.
SOURCE: Yakugaku Zasshi (1952), 72, 518-20
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 46, 1714c. -Quinone; p-O:C6H4:NNHC(:NH)NH2.HNO3;
p-C6H4[:NNHC(:NH)NH2.HNO3]2; p-toluquinone; 2,4-Me(O:)C6H3:NNHC(:NH)NH2.HNO3; 2,1,4-MeC6H3[:NNHC(:NH)NH2.HNO3]2;
 α -naphthoquinone (I); 1,4-O:C10H6:NNHC(:NH)NH2.HNO3;
1,4-C10H6[:NNHC(:NH)NH2.HNO3]2; thymoquinone and its diaminoguanylhydrazone nitrate; 2-methyl-5-methoxyquinone; anthraquinone derivs. including chrysophanol purpurin, anthrachrysone, rufigallic acid, emodic acid, and endocrocin; α -benzildioxime; salicylaldoxime; o-HOC9H6N (II); PhN(NO)ONH4; and phenanthraquinone (III) were tested for mold-preventing action in soy sauce. I and II showed about the same degree of activity as that of p-HOC6H4CO2Pr used as a control; III prevented the growth of mold for 42.5 days at the concentration of 0.001%, 51.5 days at 0.003%, and 77 days at 0.005% in contrast to the control which prevented the growth of mold for 77 days at the concentration of 0.01%. Other compds. were ineffective.

IT 106-51-4, p-Benzoquinone 553-97-9, p-Toluquinone
(as fungicides in soy sauce)
RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 553-97-9 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



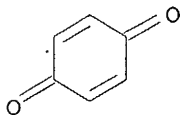
L25 ANSWER 35 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1952:23744 HCAPLUS
 DOCUMENT NUMBER: 46:23744
 ORIGINAL REFERENCE NO.: 46:4057f-h
 TITLE: Fungistatic potencies of some fluorinated p-quinones
 AUTHOR(S): Tehon, Leo R.
 CORPORATE SOURCE: Illinois State Nat. History Survey, Urbana
 SOURCE: Science (Washington, DC, United States) (1951), 114, 663-4
 CODEN: SCIEAS; ISSN: 0036-8075
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB In order to compare the effects of fluorinated quinones with those of quinones containing other halogens, bioassays according to the method of Peterson (Phytopathology 31, 1108(1941)) were carried out on 2-fluoro-1, 4-quinone, 2, 5-difluoro-1, 4-quinone (I), 2-fluoro-5-chloro-1, 4-quinone, 2-fluoro-5-bromo-1, 4-quinone, and 2-fluoro-5-methyl-1, 4-quinone (II). The test fungus presumably was a subtransplant of the strain of *Macrosporium sarcinaeforme* used by McCallan (Cornell University Agr. Experiment Sta., Mem. Number 128). Readings of spore germination were made after incubating 20 hrs., averaging the values obtained from 4 replicates. Most effective in preventing germination of spores was I. Methylation, as in II, appeared to diminish toxicity appreciably. In general the effective dosages for fluorinated quinones are remarkably low.

IT 106-51-4, p-Benzoquinone
 (fluorinated derivs., fungistatic potencies of)

RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 36 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1951:22830 HCAPLUS
 DOCUMENT NUMBER: 45:22830
 ORIGINAL REFERENCE NO.: 45:4002e-f
 TITLE: Antifungal agents and antimycotic therapy
 AUTHOR(S): Stedman, Russell L.
 CORPORATE SOURCE: McNeil Labs., Inc., Philadelphia, PA
 SOURCE: Bull. Natl. Formulary Comm. (1950), 18, 153-75
 DOCUMENT TYPE: Journal

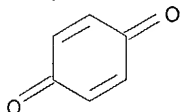
LANGUAGE: Unavailable

AB A review dealing with the following groups of therapeutic agents: fatty acids, older remedies consisting of dyes, organic acids, inorg. salts, and halogens, antibiotics, hormones, newer fungal agents including aldehyde, ketone, and ether derivs., phenol and cresol derivs., quinone, pyridine, quinoline, and thio derivs., chelating agents, and miscellaneous agents. 153 references.

IT 106-51-4, p-Benzoquinone
(derivs., **fungicidal** action of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



=>